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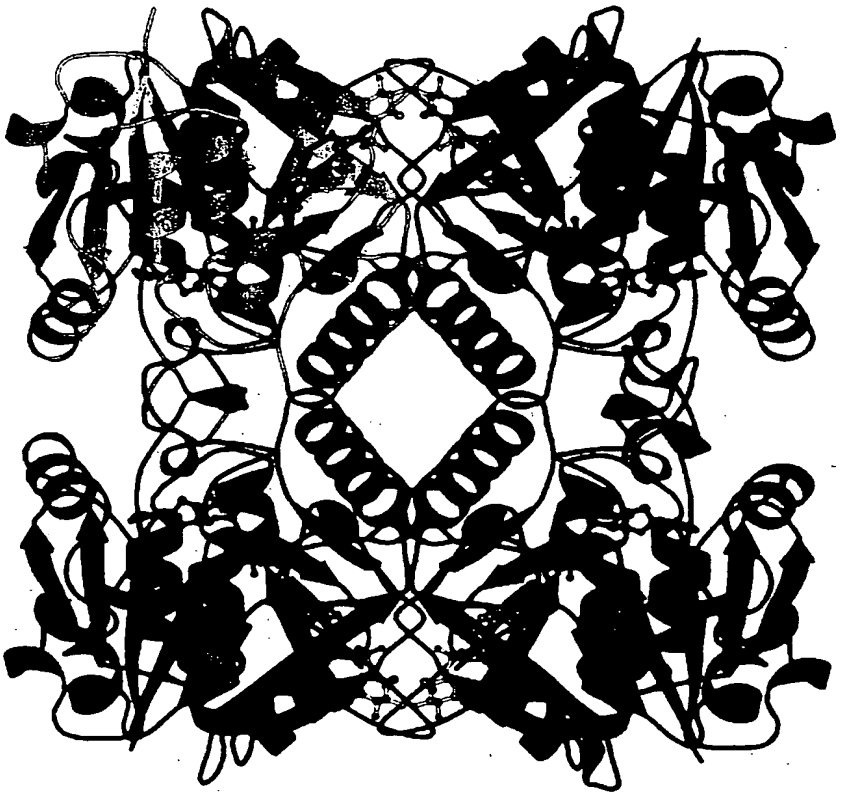
(54) Title: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE AND METHOD FOR SELECTING INHIBITORS THEREOF



(57) Abstract: There is provided a method of obtaining selecting agents which inhibit the enzyme glucose-1-phosphate thymidylyltransferase (Rm1A) based upon analysis of a model of the active and regulatory site (s) of Rm1A and interaction therewith by a potential inhibitory agent. The invention is based upon the provision of information on the structure of Rm1A obtained through X-ray diffraction studies since a crystallised form of Rm1A was obtained for the first time. The purified and crystallised from of Rm1A, obtained from *Psemdomononas aeruginosa* is also described.

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Glucose-1-Phosphate Thymidylyltransferase and Method for selecting inhibitors thereof

The present invention relates to the enzyme glucose-1-phosphate thymidylyltransferase (RmlA) and its use in a method of selecting for agents which inhibit the enzyme glucose-1-phosphate thymidylyltransferase (RmlA).

Bacterial cell-surface glycoconjugates are essential for survival of pathogenic bacteria and for interactions between bacteria and the host. Consequently, there is reason to believe that inhibitors directed against target reactions in assembly of the cell-surfaces glycoconjugates may provide viable alternate therapeutic approaches. However, bacterial cell-surface glycoconjugates show remarkable structural diversity due to variations of the sugar components, linkages and substitutions. A successful strategy requires identification of enzymes and pathways unique to bacteria, yet present within a wide spectrum of bacterial species. One

such target is the synthesis of the activated form of L-rhamnose, dTDP-L-rhamnose.

L-rhamnose is a 6-deoxyhexose that is found in the cell wall of many pathogenic microorganisms. In Gram-negative bacteria it is one of the important residues of the O-antigen of lipopolysaccharide, a factor which is a key determinant for the virulence of these species. In *Pseudomonas aeruginosa*, this sugar is a constituent of the core oligosaccharide and serves as the receptor for O-antigen polymer (Rahim *et al.*, 2000). Gram-positive bacteria such as streptococci and mycobacteria, on the other hand, utilise L-rhamnose in the arabinogalactan (AG) that attaches the lipid mycolic acid layer to the peptidoglycan layer (McNeil *et al.*, 1990). It has been demonstrated that this attachment is of vital importance to mycobacteria: inhibitors of the formation of the arabinan portion of AG, *e.g.* ethambutol, can stop cell growth and are effective drugs (see for example Deng *et al.*, 1995). As L-rhamnose is not found in mammals inhibition of its biosynthetic pathway is a target of interest in the development of novel antibiotics.

Four enzymes, glucose-1-phosphate thymidylyltransferase (RmlA), dTDP-D-glucose 4,6-dehydratase (RmlB), dTDP-6-deoxy-D-xylo-4-hexulose (RmlC) and dTDP-6-deoxy-L-lyxo 4-hexulose-4-reductase (RmlD) are required for the synthesis of dTDP-L-rhamnose from α-D-glucose-1-phosphate (G1P) and dTTP.

Significantly, these proteins are highly conserved amongst microorganisms (see for example Ma *et al.*, 1997; Graninger *et al.*, 1999) and therefore conclusions drawn from the structure of a protein from one species will have strong implications for the corresponding enzyme of another origin.

Pseudomonas aeruginosa is a Gram-negative bacterium that colonises many children with cystic fibrosis where it is a significant cause of morbidity and mortality. In addition it is an opportunistic pathogen that can cause a wide variety of infections, particularly in victims of severe burns and in patients who are for any reason immunosuppressed. This makes *Pseudomonas aeruginosa* one of the most prevalent pathogens in hospital-acquired infections. Due to its high resistance to antibiotics it is a particularly dangerous pathogen and any approach towards its control is highly sought.

RmlA (glucose-1-phosphate thymidylyltransferase, E.C. 2.2.7.24) catalyses the first of four steps in the transformation of glucose-1-phosphate (G1P) to 2'-deoxy-thymidylyl-diphospho-L-rhamnose (dTDP-L-rhamnose or dTDP-Rha) in a Mg^{2+} dependent manner (see Figure 1). The reaction product, 2'-deoxy-thymidylyl-diphospho-D-glucose (dTDP-Glc), can also be back-pyrophosphorylysed by RmlA, yielding 2'-deoxy-thymidylyl-triphosphate (dTTP) and G1P. It has been demonstrated that the enzymatic activity of RmlA is allosterically regulated by dTDP-Rha (Melo &

Glaser, 1965), making the protein a key player in the biosynthesis of rhamnose. Hence, it presents itself as an attractive target in the development of novel antibiotics.

RmlA is of particular interest as it is not only involved in the biosynthesis of L-rhamnose but also in the pathways leading to other 6-deoxy sugars such as L-talose or D-fucose as these share common intermediates in the conversion of D-glucose to their end-products (Nakano *et al.*, 2000; Yoshida *et al.*, 1999). The enzyme is highly homologous to other bacterial sugar nucleotide transferases (e.g. glucose-1-phosphate uridylyltransferase). The sugar nucleotide transferases catalyse the first step in all sugar nucleotide chemistry and are of key importance in biology and biotechnology. As RmlA shows no sequence relationship to any protein structure currently deposited in the PDB (Sussman *et al.*, 1998), it is expected to contain a novel fold. It is not yet fully clear which reaction mechanism RmlA and related enzymes follow. They may either obey Theorell-Chance (Theorell & Chance, 1951) or ordered sequential bi-bi kinetics with the nucleotide triphosphate binding to the protein first (Paule & Preiss, 1971). An oxygen of G1P's phosphate group is then believed to carry out a nucleophilic attack on the NTP α-phosphate group directly as has been demonstrated by the inversion of stereochemistry on thiosubstituted NTPs (Sheu & Frey, 1978; Figure 1).

Purification and crystallisation of RmlA enzymes from various micro-organisms has been generally possible but the crystals obtained proved to be of insufficient quality for structural studies, such as X-ray diffraction studies. Surprisingly, it has now been found that it is possible to obtain crystals of RmlA from *Pseudomonas aeruginosa*, and that crystals are of sufficient quality to perform structural studies.

The present invention provides a purified and crystallised form of RmlA from *Pseudomonas aeruginosa* and its X-ray structure.

The present invention further provides a method of selecting agents which inhibit the enzyme glucose-1-phosphate thymidylyltransferase (RmlA), said method comprising the steps of:

a) providing a model of the active or regulatory site(s) of RmlA;

b) reviewing the structure of a potential inhibitory agent for at least one of these sites; and

c) analysing the potential interaction of said agent in said site(s).

Optionally, said model may be in the form of a computer data or graphic file, and will usually be

based upon the X-ray crystal co-ordinates of RmlA. Numerous computer programs, including graphic programs, now exist to facilitate the handling of said X-ray crystal co-ordinates and mention may be made of FRODO (version 0), Insight and SYBIL, and the like.

Conveniently, the potential inhibitory agent may itself be reviewed in the form of a model, for example a computer data file. Thus, the interaction between the enzyme and potential inhibitory agent can be analysed through interaction of the models, and conveniently may be calculated by computer.

The structure of the agent to be tested for RmlA inhibitory activity may conveniently likewise be reviewed and analysed in the form of X-ray crystal co-ordinates or approximations thereof. Optionally, the potential intermolecular interaction between the agent under test and the active site of RmlA will be analysed with the aid of a computer.

In a further embodiment, the present invention provides a method of selecting an anti-microbial (such as anti-bacterial or anti-fungal) compound, said method comprising following the steps a) to c) outlined above, and including the step of selecting an agent that binds to an active or regulatory site of RmlA sufficiently tightly to impede the biosynthesis of rhamnose and thus growth of the micro-organism. It is preferred that the anti-

microbial agent is particularly effective against *Pseudomonas aeruginosa*.

In a preferred embodiment, the agent will include one or more regions able to interact with one or more of the amino acids of the active or regulatory sites (and in particular the amino acids specifically mentioned in the description of the active and regulatory sites given below and in Figures 7 and 8) to impede the biosynthesis of rhamnose.

For example, the agent may desirably comprise a negative charge and the interaction with the active site of RmlA will desirably include an association between the negative charge of the agent and at least one of the amino acids Arg 15 and Lys 25.

The agent may also be provided with thymidyl-like moiety able to interact (e.g. form hydrogen bonds) with Gly 10, Gln 82 and/or Gly 87.

The agent may also be provided with a glucose-like moiety able to interact (e.g. form hydrogen bonds) with Asn 111, Gly 146, Glu 161, Val 172 and/or Tyr 176.

The present invention will now be further described with reference to the examples and figures in which:

Figure Legends

Figure 1: Shows the first step of the conversion of glucose-1-phosphate (G1P) into 2'-deoxy-thymidylyl-diphospho-L-rhamnose or DTP-L-rhamnose. The reaction catalysed by RmlA transforms G1P and dTTP to dTDP-D-glucose.

Figure 2: Is a photograph of RmlA crystals obtained. These crystals have been grown in the presence of dTMP.

Figure 3: κ=180º section of the self-rotation search in the TMP dataset. Done with REPLACE (Tong & Rossmann, 1997). Search angle: polar XYK; orthogonalisation AXABZ

Figure 4: Table 1: Data collection statistics for non-Se-labelled RmlA crystals.

Figure 5: Table 2: Data collection statistics for MAD experiment on BM14.

Figure 6: Overall structure of the RmlA tetramer with the location of active (dark) and regulatory (light) binding site indicated by bound ligand. The bound molecule is dTDP-Glc in all cases.

Figure 7: Interactions of dTDP-Glc in the active center of RmlA. The hydrogen bonding network is indicated by dashed lines. Hydrophobic contacts are shown as lunes. Water residues are presented as cyan spheres.

Figure 8: Interactions of dTDP-Glc in the regulatory binding site of RmlA.

Examples

RmlA overexpression and purification

The open reading frame of the gene encoding RmlA from *Pseudomonas aeruginosa* was amplified using PCR with primers that incorporated a 5' *Nco*I and a 3' *Bam*HI site to facilitate cloning into a modified pET23a(+) vector (Newton & Mangroo, 1999). The plasmid also contained a sequence coding for a 6xHis-tag on the N-terminus of RmlA to allow an easy purification on metal chelating columns. Expression involves the IPTG (isopropyl-β-D-thiogalactoside)-inducible T7 promotor and ribosome-binding sites conferred by the vector. The sequence of the amplified and cloned gene was confirmed to be identical to the chromosomal copy excepting the N-terminal 6xHis-tag.

In order to overexpress RmlA *E. coli* BL21(λDE3) cells transformed with the plasmid were grown at 310 K in Luria-Bertani medium containing 100 $\mu g\ ml^{-1}$ ampicillin until the OD_{600} reached 0.6 - 0.8. Expression of the protein was then induced by addition of 1 mM IPTG. After further 3 h of culture cells were harvested by centrifugation (20 min, 6,000 g, 277 K).

The cell pellet was resuspended in a lysis buffer containing 20 mM Tris-HCl pH 8.5, 100 mM NaCl, 2 mM DTT, 5 mM PMSF and 100 μg ml^{-1} hen egg white lysozyme. After 30 min incubation at room temperature, the viscosity of the mixture was decreased by the addition of DNAse I (20 μg ml^{-1}) and by sonication (five cycles of 1 min interrupted by 1 min periods on ice). The suspension was centrifuged at 20,000 g and 277 K for 20 min and the supernatant then brought to 20 % ammonium sulfate saturation. After incubation on ice for 1 h a second centrifugation (20 min, 20,000 g, 277 K) was carried out and the supernatant then dialysed against two changes of 1 litre 20 mM Tris-HCl pH 7.0, 20 mM imidazole and 500 mM NaCl. The filtered protein solution was passed through a POROS-MC column which had been pre-loaded with nickel sulphate. Proteins were eluted with a 20 to 500 mM imidazole gradient. A protein with a molecular weight corresponding to RmlA (~ 34 kDa) was found in a peak eluting at approx. 200 mM imidazole. Fractions corresponding to this peak were pooled, concentrated with a 10 kDa cut-off Amicon membrane and dialysed against two changes of 1 litre of 20 mM Tris-HCl pH 8.5 at 277 K containing 10 mM EDTA in the first change to remove contaminating nickel ions. For further purification the protein was applied to a POROS-HQ anion exchange column on a BioCAD 700E Workstation. Elution was achieved with a 50 to 1000 mM NaCl gradient. RmlA eluted at a salt concentration of 200 mM. Pooled fractions were brought to a protein concentration of approx. 4 mg

ml^{-1} as determined by Bradford assay (Bradford, 1977) using bovine serum albumin as standard and then dialysed against two changes of 50 mM Tris-HCl pH 7.5 at 277 K. Prior to crystallisation experiments DTT was added to 4 mM and the solution filtered through a 0.2 µm membrane. This procedure typically yielded 30 mg of pure protein per litre of bacterial culture. Small aliquots of the purified protein could be stored at 255 K without deterioration for several months without addition of cryoprotecting agents. Selenomethionine labelling of *Pseudomonas aeruginosa* RmlA could not be achieved in *met*$^-$ B834(λDE3) *E. coli* cells. Under all conditions tested the protein formed inclusion bodies. Selenomethionine enriched protein was therefore produced by inhibition of the methionine biosynthesis pathway in *E. coli* BL21(λDE3) (Doublie, 1997). Briefly, cells were grown in M9 medium (64 g l^{-1} $Na_2HPO_4 \cdot 7\ H_2O$, 15 g l^{-1} KH_2PO_4, 2.5 g l^{-1} NaCl; 5 g l^{-1} NH_4Cl, 1 mM $MgSO_4$, 0.4 % glucose, 0.1 mM $CaCl_2$) at 310 K until OD_{600} reached 0.6. At this stage the amino acids lysine, phenylalanine and threonine were added to final concentrations of 100 mg l^{-1} and isoleucine, leucine and valine to 50 mg l^{-1}. Seleno-L-methionine was added to a concentration of 60 mg l^{-1}. The temperature was lowered to 303 K and the culture left to shake for further 15 min before protein overexpression was induced with 1 mM IPTG. After 6 h cells were harvested and lysed as described above. 13 mg pure protein per litre of culture could be isolated.

Protein analysis

Following the two HPLC steps, the protein appeared to be pure as judged by a SDS silver nitrate stained gel (single band at an apparent molecular weight of 34 kDa); the calculated molecular weight based on sequence being 33773 Da. A single peak with a molecular weight of 33803 Da was found in the MALDI mass spectrum. Dynamic light-scattering results (DynaPro 801) indicated the native protein to be monodisperse with a molecular weight in the range of 106 to 122 kDa indicative of a trimeric or tetrameric protein. N-terminal sequencing was performed and confirmed the protein to be Rml*A*.

The efficiency of the selenomethionine labelling procedure was scrutinised by MALDI mass spectrometry. A shift of +304 Da was found for the intact labelled protein corresponding well to the predicted additional mass of 282 Da (6 methionine residues per chain). In an important and useful second check, sulfur methionine containing fragments were undetectable in the MALDI mass spectrum of a tryptic protein digest.

Rml*A* crystallisation

Initial crystallisation conditions were obtained from Screen I and II of Hampton Research (Jancarik & Kim, 1991; Cudney *et al.*, 1994) plus NaCl, PEG 6000, PEG

6000/lithium sulphate and MPD grids. The sitting drop vapour diffusion method (Ducruix & Giegé, 1992) with 4 µl of protein sample and 4 µl of precipitant at 293 K was used throughout. Crystals appeared under 27 of the initial 192 conditions, in some cases 10 min after setup. Most promising were results from the PEG 6000/lithium sulphate grid and hence these conditions were further optimised. Plate type crystals of approx. 0.3 x 0.3 x 0.05 mm size (Figure 2) were obtained after one to seven days using 9 to 12 % (w/v) PEG 6000, 0.5 M lithium sulphate and 0.1 M citrate/NaOH pH 4.6 as precipitating solution. The initial very high mosaicity of these crystals could be greatly reduced by the addition of 1 to 2 µl 10 to 50 mM G1P, dTMP or dTDP-glucose to the protein prior to crystallisation.

Data collection

A 2.2 Å resolution dataset (see Table 1, Figure 4) from a single flash frozen crystal grown in the presence of G1P was collected in-house at 110 K using a Nonius/MacScience DIP2000 imaging plate detector system. Data were recorded as 245 non-overlapping 20 min 1º oscillations. Cryoprotection was achieved by washing the crystal in mother liquor supplemented with 16 % (v/v) PEG 600 for 10 to 15 s. The oscillation images were indexed and integrated with the program MOSFLM (Leslie, 1992) and scaled with the CCP4 program SCALA (CCP4, 1994). Higher resolution datasets of crystals grown in the presence of G1P,

dTMP, dTDP-glucose or thymidine/glucose-1-phosphate/AlF_3 were measured at the ESRF-Grenoble at beamlines ID14EH1 and BM14 (Table 1). All crystals were triclinic with approximate cell parameters of a = 71 Å, b = 73 Å, c = 134 Å; α = 89.9 °, β = 81° and γ = 81°. All attempts to index or reduce the data in a higher spacegroup failed, a native Patterson map shows no non-origin peak. A majority of the crystals were actually twinned. This could only be detected from the diffraction pattern. Trial and error was used to locate single crystals for analysis. Flash-annealing with the crystal remaining in the loop (Yeh & Hol, 1998) in some cases helped to achieve a less mosaic diffraction pattern.

In addition to the datasets shown in Table 1 (figure 4) a three-wavelength MAD experiment with a selenomethionine labelled crystal that was grown in the presence of G1P was carried out at beamline BM14 of the ESRF-Grenoble. The crystal-to-detector distance was adjusted so that the outer rim of the detector area corresponded to a resolution of 2.8 Å. 730 non-overlapping 0.5º oscillations were recorded at each of three wavelengths. The three wavelengths were chosen from an EXAFS scan of the crystal to correspond to the maximum of f´´ (peak), the maximum modulus of f´ (inflection) and minimum modulus of f´ (remote). These data were indexed and integrated with DENZO and scaled with SCALEPACK (Otwinowski & Minor, 1996) and are shown in Table 2 (figure 5).

Preliminary structural characterisation

At the beginning of this study it was not clear whether native RmlA is a trimeric or a tetrameric protein. A self-rotation search of the TMP dataset with REPLACE (Tong & Rossmann, 1997) reveals three major (> 30 σ) plus several minor (approx. 10 to 15 σ) twofold axes (Figure 3). In addition, a 60º- and a 120º-rotation axis (15.4 and 14.6 σ) are found lying parallel to the major 180º-rotation axes at φ = 8º and ψ = 98º (data not shown). The interpretation of these results was greatly aided by the determination of selenium atom positions with the program SOLVE 1.17 (Terwilliger & Berentzen, 1999). Twenty-four sites were found which could easily be grouped into eight equivalent clusters of three atoms. The clusters fall into two sets of four indicating that RmlA is a tetramer and that the unit cell of the P1 crystal form contains two tetrameric molecules. The rotation superimposing the two tetramers can be described as either as a 60º-, a 120º- or a 180º-rotation axis depending on which monomer is used as a reference point. This explains the existence of major and minor twofold axes in the κ=180º self-rotation search. First, there are inter- and intra-tetramer 180º-axes lying parallel to each other. Second, in the case of exclusively intra-tetramer axes only two pairs of two monomers are superimposed while in the other the intramolecular vectors of eight protein chains contribute to the

peak in the self rotation function, leading to a stronger signal.

The asymmetric unit of the crystal contains approximately 2400 amino acid residues and has a solvent content of 51 %, corresponding to a V_M of 2.54 $Å^3$ Da^{-1} (Matthews, 1968).

A partial set of co-ordinates from *Pseudomonas aeruginosa* RmlA is listed in Annex 1. The co-ordinates are given in two sections; the first section gives all atoms up to a distance of 15 Å to the bound product in the active site; and the second section gives all atoms up to a distance of 15 Å to the bound product in the regulatory site. The data is derived from the dTDP-glucose dataset given in Figure 4 (table 1) and represent a model of excellent geometrical properties with an R-factor of 16.3% and an R_{free} of 21.8% at a resolution of 1.77 Å. The co-ordinates also contain one bound molecule of dTDP-glucose in each monomer's active centre, which can be used in computer programs for inhibitor modelling.

STRUCTURAL CHARACTERISTICS

Fold

RmlA is a 222 tetrameric molecule and its structure is represented in Fig. 6. In *Pseudomonas aeruginosa* the monomer has a chain length of 293 amino acids. The subunit's fold can be described as a single

domain αβα sandwich, meaning that a central β-sheet is covered by layers of helices from both sides. In RmlA this mixed β-sheet is seven stranded in the order 3214657 with strand 6 being antiparallel to the rest. In addition, both helical layers contain a two stranded β-sheet structure as well. Due to its tetrameric nature each monomer is in contact with two neighbouring subunits.

Binding Sites

The RmlA monomer is capable of binding two molecules of dTDP-Glc. By sequence comparison with related nucleotidyltransferases and inspection of the glucose 1-phosphate co-complex, it is possible to definitively assign the active centre to the areas around the black bound molecules in Fig. 6. The second binding site (light grey molecules in Fig. 6) is likely going to be involved in allosteric regulation of RmlA's enzymic activity.

Active Site

The active site is exclusively made up of amino acids from one monomer. Fig. 7 gives a schematic representation of the most important interactions between dTDP-Glc and the enzyme. The amino acids can be subdivided into three groups.

Group one contains the residues involved in the catalytic mechanism and in particular the formation

or pyrophosphorolysis of diphospho ester bonds. Their importance is highlighted by a high degree of conservation amongst nucleotidyltransferases. These residues are Arg15, Asp110, Lys162 and Asp225. A high degree of conservation is also observed for Lys25 (not shown in Fig. 7). The positively charged Arg15 and Lys25 are responsible of binding the β- and the γ-phosphate group of dTDP as can be concluded from an additional sulphate molecule that is bound in the active site of RmlA but not shown in Figure 7. The position of Lys25 is stabilised by a salt bridge with Asp110, another highly conserved residue in sugar nucleotidyltransferases. The importance of Lys162 in the active centre lies in binding of the phosphate group of glucose-1-phosphate. It ensures correct orientation towards dTTP for nucleophilic attack on the α-phosphate group.

Groups 2 and 3 provide specificity for thymidyl and/or glucosyl ligands, respectively. Specificity for the thymidyl moiety results from Gly10, Gln82 and Gly87 which all form hydrogen bonds with the pyrimidine ring. The glucose part of RmlA substrates is hydrogen bonded to Asn111, Gly146, Glu161, Val172 and Tyr176. Among these, the chelating interaction of Glu161's side chain will be of high importance as it can only bind to hydroxyl groups of the sugar if these are in equatorial position.

A hydrophobic patch of three leucine residues (Leu8, Leu88, Leu108) lines the active site from the bottom.

Other residues in only hydrophobic interaction are Pro85, Tyr145 and Trp223.

Regulatory Site

The second binding site for dTDP-Glc is located in the interface between two monomers (Fig. 6), hence amino acids from two subunits contribute to its formation. The residues in this binding site (Fig. 8) are not conserved in more distantly related nucleotidyltransferases. Therefore, these enzymes' allosteric control might be achieved by other mechanisms. However, glucose-1-phosphate thymidylyltransferases from other organisms will have binding sites similar to Fig. 8 as can be concluded from their amino acid sequences. It can be concluded from Fig. 8 that dTDP-Glc is not the natural ligand of this binding site as most contacts between the protein and the glucosyl moiety are mediated by water molecules whilst the remainder of the ligand shows mainly direct hydrogen bonding.

Suitable inhibitors may either bind to the active site of RmlA, acting in a competitive mode to natural substrates and being non-cleavable, or may exploit the allosteric properties of RmlA. In the case of RmlA from *Pseudomonas aeruginosa* the latter might be the preferred approach: the protein is strongly inhibited by dTDP-rhamnose, the final product of the four enzyme pathway (Melo & Glaser, 1965), possibly

by binding to the second binding site indicated in Figure 6. As rhamnose is not found in mammals, dTDP-rhamnose derived compounds might provide lesser side effects in the application as antibiotics and are potentially good candidates as suitable RmlA inhibitors.

Several methods for essaying the activity of RmlA and related enzymes in both sugar mucleotide synthesis and pyrophosphorolysis directions have been described in the literature. They are normally based on the incorporation of radioactive compounds into the reaction products and seem to be less suited for the development of new inhibitors by high throughput screening as they require a time-consuming separation of the reaction mixtures. Therefore, it is proposed to use coupled enzyme assays for drug development purposes.

In the synthesis direction, the reaction can be followed by monitoring the production of pyrophosphate using pyrophosphate dependent fructose-6-phosphate kinase (PP_i-PFK). This enzyme generates fructose-1,6-diphosphate (F-1,6-DP) from fructose-6-phosphate (F-6-P) and pyrophosphate (PP_i). F-1,6-DP is then cleaved by aldolase to yield glyceraldehyde-3-phosphate (GAP) and dihydroxyacetone phosphate (DHAP). GAP is isomerised by triosephosphate isomerase (TPI) to give a second molecule of DHAP. Finally, DHAP is reduced to glycerol-3-phosphate (G3P) by glycerophosphate dehydrogenase (GDH) in an

NADH-dependent reaction such that the production of pyrophosphate is coupled to the depletion of NADH which can be recorded by the decrease in absorption at 340 nm (O'Brien, 1976):

DTTP + G1P -----→ dTDP-Glc + PP_i (RmlA)

PP_i + F-6-P ---→ F-1,6-DP + PP_i (PP_i-PFK)

F-1,6-DP ---→ GAP + DHAP (Aldolase)

GAP ----→ DHAP (TPI)

2 DAHP + 2 NADH → 2 G3P + 2 NAD+ (GDH)

The pyrophosphorolysis direction can be monitored by following the production of G1P, which is then isomerised to glucose-6-phosphate by phosphoglucomutase (PGM) and subsequently oxidised to 6-phospho-gluconolactone (6PGL) by glucose-6-phosphate dehydrogenase (G6P-DH), thereby generating one molecule of NADPH. This can again be followed at 340 nm (Kornfeld & Glaser, 1961):

DTDP-Glc + PP_i ---→ dTTP + G1P (RmlA)

G1P ---→ G6P (PGM)

G6P + NADP+ ---→ 6PGL + NADPH (G6P-DH)

Both assays are rapid and easy to carry out.

The active and regulatory sites of RmlA and interactions with their natural substrates are further illustrated by the Figures.

Annex 1 : 22

REGULATORY SITES

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REMARK   3   FREE R VALUE TEST SET COUNT      :12192
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   All atoms                  :   46517
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 14.387
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :   0.46
REMARK   3    B22 (A**2) :  -0.19
REMARK   3    B33 (A**2) :  -0.27
REMARK   3    B12 (A**2) :   0.03
REMARK   3    B13 (A**2) :  -0.02
REMARK   3    B23 (A**2) :  -0.25
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                  (A):
REMARK   3  NULL
REMARK   3   ESU BASED ON FREE R VALUE                             (A):
REMARK   3   0.18277
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                       (A):
REMARK   3   0.12940
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):
REMARK   3   8.01924
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   DISTANCE RESTRAINTS.                        RMS     SIGMA
REMARK   3    BOND LENGTH                  (A) : 0.021 ; 0.021
REMARK   3    BOND ANGLE             (DEGREES) : 2.076 ; 2.015
REMARK   3    Torsion angles, period 1 (DEGREES) : 5.103 ; 3.000
REMARK   3    Torsion angles, period 3 (DEGREES) :16.457 ;15.000
REMARK   3    CHIRAL-CENTER RESTRAINTS   (A**3) : 0.126 ; 0.200
REMARK   3    PLANE RESTRAINT              (A) : 0.009 ; 0.020
REMARK   3    VDW repulsions               (A) : 0.232 ; 0.300
REMARK   3    Potential hbonds             (A) : 0.217 ; 0.500
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : 1.443 ; 1.500
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REMARK   3   MAIN-CHAIN ANGLE                (A**2) : 2.158 ; 2.000
REMARK   3   SIDE-CHAIN BOND                 (A**2) : 3.125 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE                (A**2) : 4.584 ; 4.500
REMARK   3
REMARK   3 ANISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS     SIGMA
REMARK   3   Rigid-bond restraints           (A**2) : 1.894 ; 2.000
REMARK   3   Sphericity; free atoms          (A**2) : 4.664 ; 2.000
REMARK   3   Sphericity; bondec atoms        (A**2) : 2.553 ; 2.000
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS.
REMARK   3
REMARK   3  TLS details
REMARK   3  Number of tls groups                  :   8
REMARK   3
REMARK   3  Number of pieces in the TLS group   1:   1
REMARK   3  From A   1 to A 292
REMARK   3  Origin for the group                  :   1
REMARK   3   69.4830  59.4220  78.9970
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0325  0.0433  0.0247 -0.0039 -0.0136 -0.0012
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6102  0.6435  0.4229 -0.1271  0.0884 -0.0867
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   0.0248 -0.0135 -0.0505  0.0232  0.0615 -0.0461  0.0207 -0.0758
REMARK   3
REMARK   3  Number of pieces in the TLS group   2:   1
REMARK   3  From B   1 to B 293
REMARK   3  Origin for the group                  :   2
REMARK   3   61.2650  33.4890  54.1360
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0294  0.0510  0.0183  0.0014  0.0082 -0.0045
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6794  0.6303  0.4419  0.1224 -0.1618 -0.1218
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0046 -0.0119  0.0109  0.0234  0.0528  0.0423 -0.0173 -0.0642
REMARK   3
REMARK   3  Number of pieces in the TLS group   3:   1
REMARK   3  From C   1 to C 292
REMARK   3  Origin for the group                  :   3
REMARK   3  100.4020  45.2900  79.2890
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0309  0.0357  0.0395  0.0126  0.0217  0.0172
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.5756  0.7497  0.6477 -0.1840  0.0581 -0.3103
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0999 -0.0112  0.0060  0.0283 -0.1071 -0.0800  0.0406  0.0887
REMARK   3
REMARK   3  Number of pieces in the TLS group   4:   1
REMARK   3  From D   1 to D 292
REMARK   3  Origin for the group                  :   4
REMARK   3   93.1810  38.1690  43.3930
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0110  0.0453  0.0536  0.0109  0.0225  0.0295
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6426  0.7184  0.8911  0.0882 -0.0950 -0.4089
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.1237 -0.0615  0.0018 -0.0411 -0.1339 -0.0574  0.0193  0.1369
REMARK   3
REMARK   3  Number of pieces in the TLS group   5:   1
REMARK   3  From E   1 to E 292
REMARK   3  Origin for the group                  :   5
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REMARK   3    42.8770   8.9030  19.5730
REMARK   3   T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0309  0.0452  0.0352  0.0089 -0.0125 -0.0200
REMARK   3   L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.6312  0.7631  0.9845  0.0814  0.0288  0.4970
REMARK   3   S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   -0.1195 -0.0434 -0.0468  0.0342  0.1311 -0.0463 -0.0408 -0.1559
REMARK   3
REMARK   3   Number of pieces in the TLS group    6:    1
REMARK   3   From F   1 to F 293
REMARK   3   Origin for the group                 :   6
REMARK   3    38.0920  17.7800 -16.3490
REMARK   3   T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0208  0.0425  0.0417  0.0034  0.0045 -0.0015
REMARK   3   L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.8800  0.3582  0.6933  0.1180  0.1354  0.1904
REMARK   3   S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   -0.0810  0.0464 -0.0329  0.0291  0.0416  0.0160 -0.0440 -0.0740
REMARK   3
REMARK   3   Number of pieces in the TLS group    7:    1
REMARK   3   From G   1 to G 292
REMARK   3   Origin for the group                 :   7
REMARK   3    71.8950  21.8640 -15.9250
REMARK   3   T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0234  0.0522  0.0272 -0.0024 -0.0109  0.0094
REMARK   3   L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.5696  0.5742  0.4250  0.0699 -0.0286 -0.0019
REMARK   3   S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   -0.0333  0.0146  0.0152 -0.0110 -0.0283  0.0204 -0.0007  0.0589
REMARK   3
REMARK   3   Number of pieces in the TLS group    8:    1
REMARK   3   From H   1 to H 292
REMARK   3   Origin for the group                 :   8
REMARK   3    71.9070  -5.2410   8.8240
REMARK   3   T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0445  0.0386  0.0064  0.0038  0.0132  0.0109
REMARK   3   L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.4837  0.7743  0.6523 -0.1036 -0.1161  0.0699
REMARK   3   S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   -0.0109 -0.0288 -0.0166  0.0049 -0.0575 -0.0486  0.0096  0.0981
REMARK   3
REMARK   3   Hydrogens have been added in the riding positions
REMARK   3
REMARK   3
REMARK   3              Scaling details
REMARK   3   Babinet"s principle for scaling has been used
REMARK   3   Bulk solvent correction based on constant value has been used
REMARK   3   Parameters for mask calculation
REMARK   3    VDW prob radii  =   1.40
REMARK   3    ION prob radii  =   0.80
REMARK   3    Shrinkage radii =   0.80
REMARK   3
HEADER    ----                                        XX-XXX-XX    xxxx
COMPND    ---
CISPEP   1 HIS A   16     PRO A   17                      0.00
CISPEP   2 HIS B   17     PRO B   18                      0.00
CISPEP   3 HIS C   16     PRO C   17                      0.00
CISPEP   4 HIS D   16     PRO D   17                      0.00
CISPEP   5 HIS E   16     PRO E   17                      0.00
CISPEP   6 HIS G   16     PRO G   17                      0.00
CISPEP   7 HIS H   16     PRO H   17                      0.00
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CISPEP   8 HIS F   17    PRO F   18                    0.00
CRYST1   71.575   73.410  134.290  89.94  80.61  80.93 P 1           1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.013971 -0.002230 -0.002368        0.00000
SCALE2      0.000000  0.013795  0.000349        0.00000
SCALE3      0.000000  0.000000  0.007550        0.00000
ATOM   6294  C   LEU B 112      68.475  34.973  54.827  1.00  9.88           C
ANISOU 6294  C   LEU B 112    1175   1368   1209     75     80      2       C
ATOM   6295  O   LEU B 112      69.411  34.350  55.217  1.00 11.66           O
ANISOU 6295  O   LEU B 112    1490   1423   1514    112     11     82       O
ATOM   6296  N   TYR B 113      68.162  35.030  53.563  1.00  9.61           N
ANISOU 6296  N   TYR B 113    1127   1258   1266     59     42     -9       N
ATOM   6298  CA  TYR B 113      68.953  34.395  52.503  1.00  7.80           C
ANISOU 6298  CA  TYR B 113     999   1040    923      4     94     26       C
ATOM   6300  CB  TYR B 113      68.065  33.564  51.581  1.00  7.86           C
ANISOU 6300  CB  TYR B 113    1027   1071    886      7    152     26       C
ATOM   6303  CG  TYR B 113      67.339  32.444  52.224  1.00  9.60           C
ANISOU 6303  CG  TYR B 113    1325   1269   1053    -43    -63     29       C
ATOM   6304  CD1 TYR B 113      66.069  32.627  52.749  1.00 11.51           C
ANISOU 6304  CD1 TYR B 113    1341   1555   1476     -4     99     21       C
ATOM   6306  CE1 TYR B 113      65.378  31.548  53.357  1.00 10.21           C
ANISOU 6306  CE1 TYR B 113    1180   1285   1413     23     46      8       C
ATOM   6308  CZ  TYR B 113      65.973  30.311  53.427  1.00 11.84           C
ANISOU 6308  CZ  TYR B 113    1573   1440   1484     -3     84     54       C
ATOM   6309  OH  TYR B 113      65.307  29.256  54.015  1.00 10.12           O
ANISOU 6309  OH  TYR B 113     946   1215   1681    158   -103    326       O
ATOM   6311  CE2 TYR B 113      67.183  30.109  52.837  1.00 11.43           C
ANISOU 6311  CE2 TYR B 113    1157   1317   1868     72   -151    158       C
ATOM   6313  CD2 TYR B 113      67.860  31.177  52.211  1.00 10.78           C
ANISOU 6313  CD2 TYR B 113    1431   1394   1271    115   -249    126       C
ATOM   6315  C   TYR B 113      69.639  35.484  51.642  1.00  7.73           C
ANISOU 6315  C   TYR B 113    1030   1027    878     43     56     33       C
ATOM   6316  O   TYR B 113      69.122  36.576  51.488  1.00  7.43           O
ANISOU 6316  O   TYR B 113    1163   1019    639     56    111     197       O
ATOM   6317  N   TYR B 114      70.843  35.209  51.135  1.00  7.30           N
ANISOU 6317  N   TYR B 114    1038    916    817     78     37     -24      N
ATOM   6319  CA  TYR B 114      71.408  36.134  50.234  1.00  7.79           C
ANISOU 6319  CA  TYR B 114     882   1085    990     69     20      22       C
ATOM   6321  CB  TYR B 114      72.075  37.313  50.967  1.00  8.84           C
ANISOU 6321  CB  TYR B 114    1069   1172   1115     76     64      44       C
ATOM   6324  CG  TYR B 114      72.428  38.431  50.016  1.00  9.10           C
ANISOU 6324  CG  TYR B 114    1248   1039   1167    -28   -201    -16       C
ATOM   6325  CD1 TYR B 114      71.472  39.349  49.662  1.00 11.13           C
ANISOU 6325  CD1 TYR B 114    1300   1304   1623    182     38     12       C
ATOM   6327  CE1 TYR B 114      71.757  40.357  48.767  1.00 10.49           C
ANISOU 6327  CE1 TYR B 114    1484   1042   1460     33     -6     56       C
ATOM   6329  CZ  TYR B 114      73.027  40.460  48.216  1.00 10.67           C
ANISOU 6329  CZ  TYR B 114    1385   1305   1363     41   -167     37       C
ATOM   6330  OH  TYR B 114      73.311  41.487  47.315  1.00 11.18           O
ANISOU 6330  OH  TYR B 114    1336   1359   1553   -239   -299     48       O
ATOM   6332  CE2 TYR B 114      74.011  39.546  48.570  1.00  7.62           C
ANISOU 6332  CE2 TYR B 114    1062    898    935    -44   -259   -116       C
ATOM   6334  CD2 TYR B 114      73.694  38.559  49.478  1.00  7.95           C
ANISOU 6334  CD2 TYR B 114    1246    731   1040     -6    -52   -122       C
ATOM   6336  C   TYR B 114      72.432  35.447  49.350  1.00  9.28           C
ANISOU 6336  C   TYR B 114    1204   1240   1080    131     53     41       C
ATOM   6337  O   TYR B 114      73.302  34.666  49.833  1.00  8.68           O
ANISOU 6337  O   TYR B 114     789   1307   1201    372    113     51       O
ATOM   6338  N   GLY B 115      72.434  35.845  48.090  1.00  8.73           N
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ANISOU 6338  N   GLY B 115     1039   1276   1000     84   -100     32       N
ATOM   6340  CA  GLY B 115      73.544  35.449  47.224  1.00  8.72           C
ANISOU 6340  CA  GLY B 115     1098   1144   1070    109    57     82       C
ATOM   6343  C   GLY B 115      73.295  35.510  45.744  1.00  7.38           C
ANISOU 6343  C   GLY B 115      896    921    985    -61     0     30       C
ATOM   6344  O   GLY B 115      72.171  35.797  45.261  1.00  9.26           O
ANISOU 6344  O   GLY B 115     1156   1243   1119    112   -74    144       O
ATOM   6345  N   HIS B 116      74.349  35.220  45.007  1.00  7.30           N
ANISOU 6345  N   HIS B 116      932    922    917     44    -5    -10       N
ATOM   6347  CA  HIS B 116      74.300  35.259  43.540  1.00  7.38           C
ANISOU 6347  CA  HIS B 116      923    986    893    104   -25     85       C
ATOM   6349  CB  HIS B 116      75.727  35.106  42.945  1.00  7.55           C
ANISOU 6349  CB  HIS B 116     1013    928    928     55    10    103       C
ATOM   6352  CG  HIS B 116      75.746  35.098  41.450  1.00  8.35           C
ANISOU 6352  CG  HIS B 116     1105   1070    996     10    41     38       C
ATOM   6353  ND1 HIS B 116      75.393  36.207  40.714  1.00  8.46           N
ANISOU 6353  ND1 HIS B 116     1206   1073    932    121    83    126       N
ATOM   6355  CE1 HIS B 116      75.484  35.904  39.425  1.00 11.58           C
ANISOU 6355  CE1 HIS B 116     1633   1464   1302   -142   -36      4       C
ATOM   6357  NE2 HIS B 116      76.029  34.697  39.306  1.00 11.15           N
ANISOU 6357  NE2 HIS B 116     1161   1704   1369     -4     4     75       N
ATOM   6359  CD2 HIS B 116      76.164  34.156  40.561  1.00  9.33           C
ANISOU 6359  CD2 HIS B 116     1144   1203   1198     69   -66     14       C
ATOM   6361  C   HIS B 116      73.386  34.229  42.935  1.00  8.57           C
ANISOU 6361  C   HIS B 116     1024   1176   1055     73   -18     97       C
ATOM   6362  O   HIS B 116      73.424  33.059  43.290  1.00  7.60           O
ANISOU 6362  O   HIS B 116      834    952   1099    171  -185    110       O
ATOM   6363  N   ASP B 117      72.503  34.689  42.016  1.00  8.98           N
ANISOU 6363  N   ASP B 117     1046   1282   1081     86   -30    101       N
ATOM   6365  CA  ASP B 117      71.577  33.796  41.357  1.00 10.33           C
ANISOU 6365  CA  ASP B 117     1230   1401   1293     75   -56     22       C
ATOM   6367  CB  ASP B 117      72.288  32.804  40.432  1.00 10.54           C
ANISOU 6367  CB  ASP B 117     1223   1471   1309    -39   -37     57       C
ATOM   6370  CG  ASP B 117      72.760  33.467  39.144  1.00 13.93           C
ANISOU 6370  CG  ASP B 117     1930   1747   1614    -23    86     51       C
ATOM   6371  OD1 ASP B 117      72.736  34.739  39.047  1.00 14.18           O
ANISOU 6371  OD1 ASP B 117     1749   1876   1759     63    54     40       O
ATOM   6372  OD2 ASP B 117      73.128  32.765  38.171  1.00 14.50           O
ANISOU 6372  OD2 ASP B 117     2369   1619   1519   -153   438    256       O
ATOM   6373  C   ASP B 117      70.566  33.127  42.295  1.00 10.52           C
ANISOU 6373  C   ASP B 117     1403   1334   1258     40   -96     70       C
ATOM   6374  O   ASP B 117      69.981  32.125  41.968  1.00 11.35           O
ANISOU 6374  O   ASP B 117     1603   1565   1142    -22  -206   -145       O
ATOM   6375  N   PHE B 118      70.325  33.724  43.461  1.00 10.07           N
ANISOU 6375  N   PHE B 118     1330   1308   1188     19   -23    -15       N
ATOM   6377  CA  PHE B 118      69.265  33.250  44.360  1.00 10.62           C
ANISOU 6377  CA  PHE B 118     1337   1348   1347    -56   -20     30       C
ATOM   6379  CB  PHE B 118      69.265  34.048  45.664  1.00  9.09           C
ANISOU 6379  CB  PHE B 118     1034   1158   1259   -117    21    -26       C
ATOM   6382  CG  PHE B 118      68.298  33.591  46.684  1.00  9.98           C
ANISOU 6382  CG  PHE B 118     1369   1144   1277     25    49    -41       C
ATOM   6383  CD1 PHE B 118      68.327  32.317  47.151  1.00 11.71           C
ANISOU 6383  CD1 PHE B 118     1659   1400   1388     23   178     61       C
ATOM   6385  CE1 PHE B 118      67.478  31.934  48.165  1.00 10.86           C
ANISOU 6385  CE1 PHE B 118     1297   1145   1683   -313   161   -107       C
ATOM   6387  CZ  PHE B 118      66.568  32.812  48.671  1.00 11.10           C
ANISOU 6387  CZ  PHE B 118     1255   1529   1430    -14   159    112       C
ATOM   6389  CE2 PHE B 118      66.565  34.096  48.281  1.00  8.70           C
ANISOU 6389  CE2 PHE B 118      957   1364    982     81    60   -100       C
ATOM   6391  CD2 PHE B 118      67.419  34.500  47.291  1.00 10.35           C
ANISOU 6391  CD2 PHE B 118      951   1393   1588   -123   128    124       C
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ATOM   6393  C    PHE B 118      67.899  33.376  43.636  1.00 11.03           C
ANISOU 6393  C    PHE B 118    1376   1421   1391     11     27    -19       C
ATOM   6394  O    PHE B 118      67.010  32.543  43.766  1.00  8.89           O
ANISOU 6394  O    PHE B 118    1283    924   1170    -61      1     13       O
ATOM   6395  N    HIS B 119      67.774  34.420  42.847  1.00 10.46           N
ANISOU 6395  N    HIS B 119    1382   1248   1343      5     51     62       N
ATOM   6397  CA   HIS B 119      66.552  34.600  42.091  1.00 12.15           C
ANISOU 6397  CA   HIS B 119    1573   1523   1517    -14    -27    -40       C
ATOM   6399  CB   HIS B 119      66.557  35.954  41.401  1.00 12.68           C
ANISOU 6399  CB   HIS B 119    1620   1448   1749     41     32   -109       C
ATOM   6402  CG   HIS B 119      66.889  35.944  39.972  1.00 18.70           C
ANISOU 6402  CG   HIS B 119    2504   2437   2162   -139     42      8       C
ATOM   6403  ND1  HIS B 119      67.827  36.827  39.463  1.00 22.72           N
ANISOU 6403  ND1  HIS B 119    2685   3073   2872   -225    -65     26       N
ATOM   6411  C    HIS B 119      66.193  33.405  41.166  1.00 11.61           C
ANISOU 6411  C    HIS B 119    1547   1433   1429      9    -35     41       C
ATOM   6412  O    HIS B 119      65.043  32.995  41.111  1.00 11.02           O
ANISOU 6412  O    HIS B 119    1259   1530   1395     94    -68     68       O
ATOM   6413  N    GLU B 120      67.174  32.888  40.461  1.00 10.93           N
ANISOU 6413  N    GLU B 120    1467   1471   1214     25    -66      6       N
ATOM   6415  CA   GLU B 120      66.991  31.725  39.622  1.00 11.64           C
ANISOU 6415  CA   GLU B 120    1478   1482   1463    -39    -22     37       C
ATOM   6417  CB   GLU B 120      68.220  31.541  38.710  1.00 11.47           C
ANISOU 6417  CB   GLU B 120    1616   1367   1374     -5     34    -74       C
ATOM   6420  CG   GLU B 120      68.367  32.582  37.606  1.00 11.87           C
ANISOU 6420  CG   GLU B 120    1568   1419   1520    -17    -16    -24       C
ATOM   6423  CD   GLU B 120      69.184  33.815  37.959  1.00 12.06           C
ANISOU 6423  CD   GLU B 120    1560   1559   1461    -96    108    -68       C
ATOM   6424  OE1  GLU B 120      69.358  34.067  39.172  1.00 10.94           O
ANISOU 6424  OE1  GLU B 120    1081   1425   1649   -231   -268    -44       O
ATOM   6425  OE2  GLU B 120      69.633  34.517  36.994  1.00 12.75           O
ANISOU 6425  OE2  GLU B 120    1713   1273   1858   -323     48    124       O
ATOM   6426  C    GLU B 120      66.738  30.447  40.463  1.00 12.14           C
ANISOU 6426  C    GLU B 120    1553   1595   1462    -76     61     -6       C
ATOM   6427  O    GLU B 120      65.936  29.598  40.062  1.00 10.95           O
ANISOU 6427  O    GLU B 120    1296   1624   1237   -177    287    -89       O
ATOM   6428  N    LEU B 121      67.438  30.322  41.604  1.00 12.30           N
ANISOU 6428  N    LEU B 121    1528   1613   1529   -105    -32     42       N
ATOM   6430  CA   LEU B 121      67.249  29.199  42.539  1.00 12.52           C
ANISOU 6430  CA   LEU B 121    1544   1641   1571   -103    -13     26       C
ATOM   6432  CB   LEU B 121      68.151  29.344  43.765  1.00 12.80           C
ANISOU 6432  CB   LEU B 121    1525   1770   1568    -76    -14     20       C
ATOM   6435  CG   LEU B 121      68.175  28.110  44.725  1.00 15.74           C
ANISOU 6435  CG   LEU B 121    2079   1908   1991    -88    -70     80       C
ATOM   6437  CD1  LEU B 121      68.778  26.950  44.030  1.00 21.04           C
ANISOU 6437  CD1  LEU B 121    2605   2649   2737     82     -4      7       C
ATOM   6441  CD2  LEU B 121      68.933  28.316  46.002  1.00 14.06           C
ANISOU 6441  CD2  LEU B 121    1921   1916   1505      9    196     85       C
ATOM   6445  C    LEU B 121      65.777  29.186  42.987  1.00 10.89           C
ANISOU 6445  C    LEU B 121    1258   1424   1454      4      0    -22       C
ATOM   6446  O    LEU B 121      65.074  28.129  42.945  1.00 11.39           O
ANISOU 6446  O    LEU B 121    1244   1362   1719    -52    205     -2       O
ATOM   6447  N    LEU B 122      65.270  30.347  43.325  1.00 10.11           N
ANISOU 6447  N    LEU B 122    1206   1325   1308    -89    -42     -4       N
ATOM   6449  CA   LEU B 122      63.826  30.466  43.703  1.00  9.01           C
ANISOU 6449  CA   LEU B 122    1042   1213   1166    -10      8     79       C
ATOM   6451  CB   LEU B 122      63.576  31.857  44.218  1.00  8.22           C
ANISOU 6451  CB   LEU B 122     826   1242   1054   -142     37     45       C
ATOM   6454  CG   LEU B 122      64.227  32.253  45.565  1.00  8.65           C
ANISOU 6454  CG   LEU B 122     982   1247   1056     -1    188    -86       C
ATOM   6456  CD1  LEU B 122      64.051  33.713  45.823  1.00  9.74           C
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ANISOU 6456  CD1 LEU B 122     1117   1199   1382    104     50    169       C
ATOM   6460  CD2 LEU B 122      63.707  31.467  46.720  1.00  9.31           C
ANISOU 6460  CD2 LEU B 122     1313   1116   1108   -102     70    113       C
ATOM   6464  C   LEU B 122      62.822  30.173  42.553  1.00 10.11           C
ANISOU 6464  C   LEU B 122     1356   1175   1310   -111     68   -105       C
ATOM   6465  O   LEU B 122      61.810  29.486  42.674  1.00  9.51           O
ANISOU 6465  O   LEU B 122      832   1369   1411    -35    -12    -23       O
ATOM   6466  N   GLY B 123      63.108  30.726  41.414  1.00 11.03           N
ANISOU 6466  N   GLY B 123     1584   1342   1264   -123     41    -73       N
ATOM   6468  CA  GLY B 123      62.290  30.499  40.249  1.00 12.07           C
ANISOU 6468  CA  GLY B 123     1532   1575   1478   -125     29     -4       C
ATOM   6471  C   GLY B 123      62.228  29.038  39.810  1.00 12.25           C
ANISOU 6471  C   GLY B 123     1673   1559   1419    -73     26     41       C
ATOM   6472  O   GLY B 123      61.135  28.604  39.406  1.00 13.28           O
ANISOU 6472  O   GLY B 123     1625   1867   1553   -189     25    -20       O
ATOM   6473  N   SER B 124      63.335  28.298  39.872  1.00 12.13           N
ANISOU 6473  N   SER B 124     1435   1717   1456   -163    105     61       N
ATOM   6475  CA  SER B 124      63.315  26.867  39.522  1.00 12.94           C
ANISOU 6475  CA  SER B 124     1629   1762   1522    -36     34     36       C
ATOM   6477  CB  SER B 124      64.666  26.237  39.634  1.00 13.63           C
ANISOU 6477  CB  SER B 124     1712   1804   1662    -70     12     55       C
ATOM   6480  OG  SER B 124      65.493  26.745  38.613  1.00 16.55           O
ANISOU 6480  OG  SER B 124     2085   2182   2019     33    101    182       O
ATOM   6482  C   SER B 124      62.375  26.135  40.476  1.00 13.37           C
ANISOU 6482  C   SER B 124     1756   1776   1547   -167     33     42       C
ATOM   6483  O   SER B 124      61.508  25.348  40.054  1.00 13.72           O
ANISOU 6483  O   SER B 124     2075   1848   1290   -232    -85   -107       O
ATOM   6484  N   ALA B 125      62.492  26.428  41.769  1.00 11.71           N
ANISOU 6484  N   ALA B 125     1465   1587   1396   -135      5    -19       N
ATOM   6486  CA  ALA B 125      61.581  25.745  42.713  1.00 11.64           C
ANISOU 6486  CA  ALA B 125     1586   1505   1331   -105     15      1       C
ATOM   6488  CB  ALA B 125      62.073  25.892  44.139  1.00 11.91           C
ANISOU 6488  CB  ALA B 125     1558   1486   1479   -152    -17    -40       C
ATOM   6492  C   ALA B 125      60.122  26.192  42.572  1.00 10.84           C
ANISOU 6492  C   ALA B 125     1498   1387   1230    -84      5     11       C
ATOM   6532  CD  ARG B 128      60.298  21.165  41.519  1.00 18.77           C
ANISOU 6532  CD  ARG B 128     2511   2444   2177   -125     28     27       C
ATOM   6535  NE  ARG B 128      61.529  20.700  40.936  1.00 21.99           N
ANISOU 6535  NE  ARG B 128     2812   2583   2959    144   -310   -156       N
ATOM   6537  CZ  ARG B 128      61.999  19.477  40.972  1.00 15.47           C
ANISOU 6537  CZ  ARG B 128     2036   2102   1740   -116   -470    -99       C
ATOM   6538  NH1 ARG B 128      61.420  18.557  41.653  1.00 14.38           N
ANISOU 6538  NH1 ARG B 128     1712   2162   1589   -277   -394     56       N
ATOM   6541  NH2 ARG B 128      63.111  19.242  40.373  1.00 17.94           N
ANISOU 6541  NH2 ARG B 128     2299   2506   2010    -56   -175    -77       N
ATOM   6596  CA  SER B 133      61.003  21.436  47.325  1.00  7.43           C
ANISOU 6596  CA  SER B 133      863   1003    957     13    -60    -44       C
ATOM   6598  CB  SER B 133      61.254  22.334  46.130  1.00  7.20           C
ANISOU 6598  CB  SER B 133      722    952   1061      9    -42     -6       C
ATOM   6601  OG  SER B 133      60.798  21.793  44.885  1.00  7.70           O
ANISOU 6601  OG  SER B 133      713   1276    936    -69   -172     17       O
ATOM   6603  C   SER B 133      61.483  22.145  48.596  1.00  7.62           C
ANISOU 6603  C   SER B 133      986    957    950     14     48    -40       C
ATOM   6604  O   SER B 133      60.831  23.068  49.081  1.00  8.09           O
ANISOU 6604  O   SER B 133      941   1173    958    -58    192   -139       O
ATOM   6605  N   VAL B 134      62.653  21.739  49.068  1.00  6.84           N
ANISOU 6605  N   VAL B 134      804    875    916     48    102   -104       N
ATOM   6607  CA  VAL B 134      63.297  22.261  50.256  1.00  6.93           C
ANISOU 6607  CA  VAL B 134      868    930    834     19     -8    -46       C
ATOM   6609  CB  VAL B 134      63.078  21.349  51.462  1.00  8.11           C
ANISOU 6609  CB  VAL B 134     1060   1036    985    -19     65    -54       C
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ATOM   6615  CG2 VAL B 134      63.850  20.005  51.357  1.00  9.68           C
ANISOU 6615  CG2 VAL B 134    1360   1156   1158   -123     20     12       C
ATOM   6619  C   VAL B 134      64.797  22.369  49.946  1.00  7.97           C
ANISOU 6619  C   VAL B 134     995   1003   1027    -43      0    -43       C
ATOM   6620  O   VAL B 134      65.247  21.827  48.978  1.00  9.70           O
ANISOU 6620  O   VAL B 134    1066   1341   1278    -36   -109   -156       O
ATOM   6621  N   PHE B 135      65.546  23.086  50.772  1.00  7.57           N
ANISOU 6621  N   PHE B 135    1017   1087    770     15    -49    -23       N
ATOM   6623  CA  PHE B 135      66.943  23.426  50.530  1.00  8.09           C
ANISOU 6623  CA  PHE B 135    1012   1097    963     73    -29      1       C
ATOM   6625  CB  PHE B 135      67.060  24.916  50.305  1.00  8.70           C
ANISOU 6625  CB  PHE B 135     832   1327   1146    -61     51     -8       C
ATOM   6628  CG  PHE B 135      66.273  25.377  49.135  1.00 10.94           C
ANISOU 6628  CG  PHE B 135    1378   1321   1455    -61    -99    -36       C
ATOM   6629  CD1 PHE B 135      64.942  25.787  49.294  1.00 14.22           C
ANISOU 6629  CD1 PHE B 135    1604   1903   1893     17      3    -14       C
ATOM   6631  CE1 PHE B 135      64.203  26.127  48.196  1.00 16.39           C
ANISOU 6631  CE1 PHE B 135    1777   2233   2218    141     77     76       C
ATOM   6633  CZ  PHE B 135      64.778  26.094  46.936  1.00 17.11           C
ANISOU 6633  CZ  PHE B 135    2309   2123   2068     20   -158     43       C
ATOM   6635  CE2 PHE B 135      66.033  25.682  46.784  1.00 15.86           C
ANISOU 6635  CE2 PHE B 135    2082   2010   1932    -51     76     89       C
ATOM   6637  CD2 PHE B 135      66.787  25.306  47.883  1.00 14.39           C
ANISOU 6637  CD2 PHE B 135    1818   1885   1763    -16     78     51       C
ATOM   6639  C   PHE B 135      67.798  22.981  51.711  1.00  8.70           C
ANISOU 6639  C   PHE B 135    1170   1129   1004     46    -36    -35       C
ATOM   6640  O   PHE B 135      67.394  23.171  52.873  1.00  9.72           O
ANISOU 6640  O   PHE B 135    1520   1230    940    -29    -39    247       O
ATOM   6641  N   ALA B 136      68.910  22.321  51.386  1.00  7.74           N
ANISOU 6641  N   ALA B 136     892   1086    961    -16    -61    100       N
ATOM   6643  CA  ALA B 136      69.870  21.847  52.388  1.00  7.69           C
ANISOU 6643  CA  ALA B 136     965    998    958     -3    -41     84       C
ATOM   6645  CB  ALA B 136      70.215  20.419  52.076  1.00  8.30           C
ANISOU 6645  CB  ALA B 136     970   1226    956     17    -65     41       C
ATOM   6649  C   ALA B 136      71.120  22.726  52.405  1.00  8.69           C
ANISOU 6649  C   ALA B 136    1163   1108   1030     -9     -2     55       C
ATOM   6650  O   ALA B 136      71.699  23.024  51.348  1.00  9.88           O
ANISOU 6650  O   ALA B 136    1248   1395   1108   -236    212     50       O
ATOM   6651  N   TYR B 137      71.562  23.103  53.600  1.00  7.61           N
ANISOU 6651  N   TYR B 137    1117   1021    750    -86     47     79       N
ATOM   6653  CA  TYR B 137      72.668  24.023  53.761  1.00  7.01           C
ANISOU 6653  CA  TYR B 137     858    959    848     50    -29      4       C
ATOM   6655  CB  TYR B 137      72.170  25.396  54.039  1.00  5.60           C
ANISOU 6655  CB  TYR B 137     660    986    481    158     64    -15       C
ATOM   6658  CG  TYR B 137      73.094  26.593  54.050  1.00  7.74           C
ANISOU 6658  CG  TYR B 137     972    916   1050    145    -45     29       C
ATOM   6659  CD1 TYR B 137      73.395  27.309  52.887  1.00  8.47           C
ANISOU 6659  CD1 TYR B 137    1084   1200    931    -20    -28    -89       C
ATOM   6661  CE1 TYR B 137      74.172  28.474  52.929  1.00  8.41           C
ANISOU 6661  CE1 TYR B 137    1046   1076   1072    -32     10     87       C
ATOM   6663  CZ  TYR B 137      74.671  28.944  54.149  1.00  7.72           C
ANISOU 6663  CZ  TYR B 137     958    897   1076    -37     91     87       C
ATOM   6664  OH  TYR B 137      75.410  30.080  54.226  1.00  8.42           O
ANISOU 6664  OH  TYR B 137     896    941   1359   -155     38   -107       O
ATOM   6666  CE2 TYR B 137      74.379  28.295  55.304  1.00  5.35           C
ANISOU 6666  CE2 TYR B 137     523    792    718    208   -123    159       C
ATOM   6668  CD2 TYR B 137      73.603  27.079  55.236  1.00  9.47           C
ANISOU 6668  CD2 TYR B 137    1184   1225   1189     64     50   -110       C
ATOM   6670  C   TYR B 137      73.600  23.560  54.864  1.00  6.91           C
ANISOU 6670  C   TYR B 137     996    881    748     -6    -54     13       C
ATOM   6671  O   TYR B 137      73.138  23.215  55.943  1.00  6.59           O
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ANISOU 6671  O   TYR B 137      916    777    810    -72    -25    -82       O
ATOM   6672  N   HIS B 138    74.892  23.489  54.518  1.00  5.78           N
ANISOU 6672  N   HIS B 138      761    682    750    -84      0     46       N
ATOM   6674  CA  HIS B 138    75.898  23.030  55.456  1.00  7.38           C
ANISOU 6674  CA  HIS B 138      962    860    980   -117      5     13       C
ATOM   6676  CB  HIS B 138    77.239  22.816  54.766  1.00  7.04           C
ANISOU 6676  CB  HIS B 138      882    754   1038    -86    -53    -59       C
ATOM   6679  CG  HIS B 138    78.208  22.038  55.560  1.00  7.62           C
ANISOU 6679  CG  HIS B 138     1045   1008    841    -85     77      5       C
ATOM   6680  ND1 HIS B 138    78.874  22.569  56.641  1.00  7.25           N
ANISOU 6680  ND1 HIS B 138      698   1154    899    -97   -265     16       N
ATOM   6682  CE1 HIS B 138    79.689  21.641  57.134  1.00 10.52           C
ANISOU 6682  CE1 HIS B 138     1577   1323   1097     46    -34    -95       C
ATOM   6684  NE2 HIS B 138    79.591  20.553  56.399  1.00 10.01           N
ANISOU 6684  NE2 HIS B 138     1385    938   1480    -44     -5    188       N
ATOM   6686  CD2 HIS B 138    78.593  20.739  55.476  1.00 10.19           C
ANISOU 6686  CD2 HIS B 138     1297   1127   1448   -135    -63    -16       C
ATOM   6688  C   HIS B 138    76.043  24.035  56.579  1.00  8.16           C
ANISOU 6688  C   HIS B 138     1013    976   1110    -39    -35     -7       C
ATOM   6689  O   HIS B 138    76.275  25.202  56.340  1.00  7.93           O
ANISOU 6689  O   HIS B 138      956    838   1216   -142      0    -97       O
ATOM   6690  N   VAL B 139    75.977  23.554  57.798  1.00  8.34           N
ANISOU 6690  N   VAL B 139     1028   1039   1098   -196     33     20       N
ATOM   6692  CA  VAL B 139    76.073  24.411  58.971  1.00  9.44           C
ANISOU 6692  CA  VAL B 139     1208   1219   1160    -37     -4    -24       C
ATOM   6694  CB  VAL B 139    74.667  24.696  59.635  1.00  9.21           C
ANISOU 6694  CB  VAL B 139     1168   1183   1148    -35    -58      6       C
ATOM   6696  CG1 VAL B 139    73.811  25.510  58.743  1.00 11.13           C
ANISOU 6696  CG1 VAL B 139     1331   1479   1419     68     18     24       C
ATOM   6700  CG2 VAL B 139    73.947  23.396  60.109  1.00 11.01           C
ANISOU 6700  CG2 VAL B 139     1348   1453   1381    -95    -62    -29       C
ATOM   6704  C   VAL B 139    76.985  23.839  60.033  1.00  9.80           C
ANISOU 6704  C   VAL B 139     1299   1255   1168    -39    -23     -4       C
ATOM   6705  O   VAL B 139    77.306  22.617  60.057  1.00  9.37           O
ANISOU 6705  O   VAL B 139     1305   1253   1001      1   -149   -156       O
ATOM   6706  N   LEU B 140    77.391  24.727  60.951  1.00 10.87           N
ANISOU 6706  N   LEU B 140     1521   1324   1284    -31    -91    -36       N
ATOM   6834  N   VAL B 148    68.871  16.843  57.216  1.00  7.84           N
ANISOU 6834  N   VAL B 148      792   1137   1050     10     20     88       N
ATOM   6836  CA  VAL B 148    68.695  15.888  56.162  1.00  8.13           C
ANISOU 6836  CA  VAL B 148      958   1123   1006     27     -4     47       C
ATOM   6838  CB  VAL B 148    68.232  16.534  54.839  1.00  8.35           C
ANISOU 6838  CB  VAL B 148     1031   1112   1027     41    -40     28       C
ATOM   6840  CG1 VAL B 148    69.264  17.584  54.296  1.00  9.93           C
ANISOU 6840  CG1 VAL B 148     1371   1201   1197      0   -119     -2       C
ATOM   6844  CG2 VAL B 148    67.975  15.422  53.760  1.00  9.54           C
ANISOU 6844  CG2 VAL B 148     1275   1213   1135     87    -49    118       C
ATOM   6848  C   VAL B 148    69.972  15.066  55.962  1.00  8.79           C
ANISOU 6848  C   VAL B 148     1135   1173   1030     20      0    -24       C
ATOM   6849  O   VAL B 148    71.100  15.607  55.875  1.00  8.58           O
ANISOU 6849  O   VAL B 148      977   1237   1042     99    -62    -43       O
ATOM   6850  N   GLU B 149    69.769  13.761  55.881  1.00  8.38           N
ANISOU 6850  N   GLU B 149     1104   1038   1039     33    -84     48       N
ATOM   6852  CA  GLU B 149    70.837  12.781  55.604  1.00  8.67           C
ANISOU 6852  CA  GLU B 149     1179   1126    990     82     81      2       C
ATOM   6863  C   GLU B 149    70.737  12.254  54.186  1.00  7.88           C
ANISOU 6863  C   GLU B 149     1057    937    998     34     39     -6       C
ATOM   6864  O   GLU B 149    69.651  12.080  53.659  1.00  7.98           O
ANISOU 6864  O   GLU B 149      866    976   1186    139    238   -174       O
ATOM   6865  N   PHE B 150    71.900  12.097  53.536  1.00  7.34           N
ANISOU 6865  N   PHE B 150      767   1051    969    117     -7     31       N
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ATOM   6867  CA  PHE B 150      71.969  11.579  52.168  1.00  7.78           C
ANISOU 6867  CA  PHE B 150      941   1007   1005     26     -8    -15       C
ATOM   6869  CB  PHE B 150      72.739  12.540  51.231  1.00  7.97           C
ANISOU 6869  CB  PHE B 150     1032   1064    933     28     -2     -2       C
ATOM   6872  CG  PHE B 150      72.173  13.948  51.206  1.00  8.57           C
ANISOU 6872  CG  PHE B 150     1195    938   1120     45    -41     93       C
ATOM   6873  CD1 PHE B 150      72.557  14.895  52.134  1.00 12.11           C
ANISOU 6873  CD1 PHE B 150     1643   1428   1531     22   -203     54       C
ATOM   6875  CE1 PHE B 150      72.003  16.216  52.140  1.00 10.64           C
ANISOU 6875  CE1 PHE B 150     1351   1173   1516   -115   -139    -97       C
ATOM   6877  CZ  PHE B 150      71.046  16.534  51.256  1.00 10.18           C
ANISOU 6877  CZ  PHE B 150     1334   1242   1290   -130     40    -33       C
ATOM   6879  CE2 PHE B 150      70.623  15.549  50.351  1.00 11.13           C
ANISOU 6879  CE2 PHE B 150     1491   1469   1268     38   -131   -124       C
ATOM   6881  CD2 PHE B 150      71.171  14.282  50.341  1.00 10.74           C
ANISOU 6881  CD2 PHE B 150     1347   1344   1386    -85   -161     29       C
ATOM   6883  C   PHE B 150      72.700  10.265  52.100  1.00  8.82           C
ANISOU 6883  C   PHE B 150     1038   1171   1142     64    -21     63       C
ATOM   6884  O   PHE B 150      73.608  10.019  52.917  1.00  8.69           O
ANISOU 6884  O   PHE B 150      998   1272   1031    219   -107    -17       O
ATOM   6885  N   ASP B 151      72.365   9.462  51.099  1.00  7.95           N
ANISOU 6885  N   ASP B 151      855   1103   1063     54    -26    -36       N
ATOM   6887  CA  ASP B 151      73.146   8.247  50.874  1.00 11.66           C
ANISOU 6887  CA  ASP B 151     1462   1489   1478     -6     46      0       C
ATOM   6893  OD1 ASP B 151      72.308   8.468  48.189  1.00 14.12           O
ANISOU 6893  OD1 ASP B 151     2159   1645   1560   -238   -102   -219       O
ATOM   6895  C   ASP B 151      74.422   8.605  50.100  1.00 12.63           C
ANISOU 6895  C   ASP B 151     1537   1674   1588    -69     97    -21       C
ATOM   6896  O   ASP B 151      74.642   9.780  49.779  1.00 12.87           O
ANISOU 6896  O   ASP B 151     1663   1654   1569    -70    101    -32       O
ATOM   6897  N   GLN B 152      75.215   7.600  49.759  1.00 14.56           N
ANISOU 6897  N   GLN B 152     1777   1810   1944     32      9    118       N
ATOM   6899  CA  GLN B 152      76.488   7.838  49.037  1.00 17.68           C
ANISOU 6899  CA  GLN B 152     2162   2279   2274     14     76      1       C
ATOM   6912  C   GLN B 152      76.263   8.376  47.652  1.00 17.50           C
ANISOU 6912  C   GLN B 152     2171   2225   2250     72     32     10       C
ATOM   6913  O   GLN B 152      77.173   8.900  47.045  1.00 19.80           O
ANISOU 6913  O   GLN B 152     2439   2641   2443    139    -13     43       O
ATOM   6914  N   GLY B 153      75.053   8.272  47.131  1.00 18.53           N
ANISOU 6914  N   GLY B 153     2378   2348   2312     57     43    -40       N
ATOM   6916  CA  GLY B 153      74.773   8.831  45.820  1.00 18.90           C
ANISOU 6916  CA  GLY B 153     2436   2448   2296     84     37    -55       C
ATOM   6919  C   GLY B 153      74.248  10.248  45.806  1.00 19.41           C
ANISOU 6919  C   GLY B 153     2552   2497   2323     34     25     20       C
ATOM   6920  O   GLY B 153      74.055  10.805  44.731  1.00 20.09           O
ANISOU 6920  O   GLY B 153     2598   2890   2145    145     11    -51       O
ATOM   6921  N   GLY B 154      74.036  10.850  46.984  1.00 18.63           N
ANISOU 6921  N   GLY B 154     2469   2370   2237     28     46    -33       N
ATOM   6923  CA  GLY B 154      73.537  12.212  47.068  1.00 18.75           C
ANISOU 6923  CA  GLY B 154     2451   2422   2248    -18     -6    -15       C
ATOM   6926  C   GLY B 154      72.049  12.274  47.245  1.00 18.31           C
ANISOU 6926  C   GLY B 154     2411   2345   2198     15     10     -8       C
ATOM   6927  O   GLY B 154      71.453  13.346  47.239  1.00 20.30           O
ANISOU 6927  O   GLY B 154     2655   2699   2358     82     11    -60       O
ATOM   6928  N   LYS B 155      71.425  11.117  47.411  1.00 17.75           N
ANISOU 6928  N   LYS B 155     2314   2317   2110     37     12    -80       N
ATOM   6930  CA  LYS B 155      69.988  11.059  47.555  1.00 17.17           C
ANISOU 6930  CA  LYS B 155     2180   2237   2103     91     28    -17       C
ATOM   6932  CB  LYS B 155      69.482   9.761  47.002  1.00 17.96           C
ANISOU 6932  CB  LYS B 155     2303   2430   2091    -12    -30    -48       C
ATOM   6935  CG  LYS B 155      67.966   9.620  47.005  1.00 21.83           C
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ANISOU 6935  CG  LYS B 155     2640   2916   2737     15     77     -3       C
ATOM   6948  C   LYS B 155      69.559  11.180  49.042  1.00 15.76           C
ANISOU 6948  C   LYS B 155     2059   2050   1878    124    -21    -73       C
ATOM   6949  O   LYS B 155      70.065  10.465  49.938  1.00 14.36           O
ANISOU 6949  O   LYS B 155     1609   1920   1924    334   -186   -205       O
ATOM   6950  N   ALA B 156      68.603  12.075  49.285  1.00 13.95           N
ANISOU 6950  N   ALA B 156     1638   1987   1674    152    -62    -70       N
ATOM   6952  CA  ALA B 156      68.012  12.259  50.637  1.00 13.87           C
ANISOU 6952  CA  ALA B 156     1728   1857   1685     94    -29    -28       C
ATOM   6954  CB  ALA B 156      66.884  13.323  50.575  1.00 13.88           C
ANISOU 6954  CB  ALA B 156     1673   1783   1815     19    -75    -91       C
ATOM   6958  C   ALA B 156      67.393  10.975  51.100  1.00 13.28           C
ANISOU 6958  C   ALA B 156     1610   1744   1690    112    -29   -165       C
ATOM   7147  CA  SER B 168      74.913  15.048  58.788  1.00  8.49           C
ANISOU 7147  CA  SER B 168      964   1151   1110      2    -31    -32       C
ATOM   7149  CB  SER B 168      74.321  15.086  57.392  1.00  7.62           C
ANISOU 7149  CB  SER B 168      888   1013    992    -25    -44   -109       C
ATOM   7152  OG  SER B 168      73.281  16.077  57.307  1.00  8.98           O
ANISOU 7152  OG  SER B 168      826   1444   1140     53   -406   -271       O
ATOM   7154  C   SER B 168      75.000  16.498  59.258  1.00  8.20           C
ANISOU 7154  C   SER B 168      925   1116   1075     27    -72    -66       C
ATOM   7156  N   ASN B 169      75.720  17.311  58.516  1.00  8.34           N
ANISOU 7156  N   ASN B 169     1082   1134    953     33    -28     12       N
ATOM   7158  CA  ASN B 169      75.830  18.723  58.792  1.00  9.44           C
ANISOU 7158  CA  ASN B 169     1280   1219   1087     60     21    -29       C
ATOM   7160  CB  ASN B 169      77.288  19.190  58.675  1.00 10.02           C
ANISOU 7160  CB  ASN B 169     1439   1222   1145      1    -50    -65       C
ATOM   7163  CG  ASN B 169      78.135  18.686  59.862  1.00 11.94           C
ANISOU 7163  CG  ASN B 169     1572   1549   1415     80   -166   -103       C
ATOM   7165  ND2 ASN B 169      79.280  18.144  59.581  1.00 10.28           N
ANISOU 7165  ND2 ASN B 169     1387   1439   1079      3   -271    -63       N
ATOM   7168  C   ASN B 169      74.902  19.558  57.911  1.00  9.68           C
ANISOU 7168  C   ASN B 169     1384   1215   1077    -22    -80    -15       C
ATOM   7169  O   ASN B 169      75.076  20.779  57.793  1.00 10.98           O
ANISOU 7169  O   ASN B 169     1808   1180   1180   -171    -94    -73       O
ATOM   7170  N   TYR B 170      73.947  18.924  57.249  1.00  8.76           N
ANISOU 7170  N   TYR B 170     1193   1035   1100    -16     82    -62       N
ATOM   7172  CA  TYR B 170      73.041  19.648  56.357  1.00  6.97           C
ANISOU 7172  CA  TYR B 170      859    947    839    -65     20    -13       C
ATOM   7174  CB  TYR B 170      72.838  18.873  55.047  1.00  7.14           C
ANISOU 7174  CB  TYR B 170      744   1100    869     27     64    -56       C
ATOM   7177  CG  TYR B 170      74.049  19.087  54.169  1.00  6.20           C
ANISOU 7177  CG  TYR B 170      682    865    806    -82     28     84       C
ATOM   7178  CD1 TYR B 170      75.125  18.210  54.227  1.00  7.09           C
ANISOU 7178  CD1 TYR B 170      881   1015    797    -42    -24    -21       C
ATOM   7180  CE1 TYR B 170      76.267  18.445  53.502  1.00  6.23           C
ANISOU 7180  CE1 TYR B 170      789    825    751    -21     92    -81       C
ATOM   7182  CZ  TYR B 170      76.319  19.611  52.703  1.00  8.76           C
ANISOU 7182  CZ  TYR B 170     1264   1229    833    -31   -143    -45       C
ATOM   7183  OH  TYR B 170      77.437  19.928  51.984  1.00 10.49           O
ANISOU 7183  OH  TYR B 170     1549   1362   1073   -217     90    -84       O
ATOM   7185  CE2 TYR B 170      75.288  20.489  52.678  1.00  8.94           C
ANISOU 7185  CE2 TYR B 170     1111   1124   1159    -72    148    -78       C
ATOM   7187  CD2 TYR B 170      74.161  20.230  53.421  1.00  7.63           C
ANISOU 7187  CD2 TYR B 170     1007    924    965    -99     42    -17       C
ATOM   7189  C   TYR B 170      71.705  19.966  56.998  1.00  8.15           C
ANISOU 7189  C   TYR B 170      980   1052   1062    -14      4     -7       C
ATOM   7190  O   TYR B 170      70.939  19.041  57.332  1.00  9.22           O
ANISOU 7190  O   TYR B 170     1159   1096   1248   -254    192    159       O
ATOM   7191  N   ALA B 171      71.437  21.251  57.213  1.00  7.85           N
ANISOU 7191  N   ALA B 171      922    915   1145    -85     -3    128       N
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ATOM   7193  CA  ALA B 171      70.157  21.703  57.779  1.00  6.04           C
ANISOU 7193  CA  ALA B 171      830    722    741    -16     -7    129       C
ATOM   7195  CB  ALA B 171      70.345  23.032  58.562  1.00  7.20           C
ANISOU 7195  CB  ALA B 171      910    977    845     34   -101    113       C
ATOM   7199  C   ALA B 171      69.182  21.939  56.641  1.00  7.69           C
ANISOU 7199  C   ALA B 171      914   1065    940    -10    -11     60       C
ATOM   7200  O   ALA B 171      69.585  22.371  55.569  1.00  9.49           O
ANISOU 7200  O   ALA B 171     1245   1401    958     41    -59     75       O
ATOM   7201  N   VAL B 172      67.904  21.754  56.929  1.00  7.02           N
ANISOU 7201  N   VAL B 172      877    941    849    -86     37     83       N
ATOM   7203  CA  VAL B 172      66.820  22.038  55.994  1.00  7.98           C
ANISOU 7203  CA  VAL B 172      986   1067    978     -7     60     93       C
ATOM   7205  CB  VAL B 172      65.689  21.006  56.048  1.00  7.69           C
ANISOU 7205  CB  VAL B 172      860    985   1074     13     10     81       C
ATOM   7207  CG1 VAL B 172      64.547  21.391  55.088  1.00  7.84           C
ANISOU 7207  CG1 VAL B 172     1162   1028    787   -190    -64    125       C
ATOM   7211  CG2 VAL B 172      66.192  19.558  55.778  1.00  8.46           C
ANISOU 7211  CG2 VAL B 172     1103   1224    887   -156    204    -81       C
ATOM   7215  C   VAL B 172      66.365  23.443  56.381  1.00  8.06           C
ANISOU 7215  C   VAL B 172      967   1038   1058    -44      8     38       C
ATOM   7217  N   THR B 173      66.585  24.394  55.469  1.00  9.20           N
ANISOU 7217  N   THR B 173     1211   1258   1024     32     28     12       N
ATOM   7219  CA  THR B 173      66.371  25.812  55.744  1.00  9.64           C
ANISOU 7219  CA  THR B 173     1185   1226   1249     26     17     75       C
ATOM   7221  CB  THR B 173      67.023  26.735  54.707  1.00  9.14           C
ANISOU 7221  CB  THR B 173     1041   1285   1147     96    122     -4       C
ATOM   7223  OG1 THR B 173      66.266  26.732  53.499  1.00 10.36           O
ANISOU 7223  OG1 THR B 173     1012   1431   1493    -10    304     28       O
ATOM   7225  CG2 THR B 173      68.470  26.306  54.352  1.00 10.18           C
ANISOU 7225  CG2 THR B 173     1304   1372   1190    -76    229    162       C
ATOM   7251  CD2 LEU B 175      63.498  29.481  49.870  1.00 12.70           C
ANISOU 7251  CD2 LEU B 175     1717   1586   1521   -282    120   -139       C
ATOM   7865  N   SER B 213      61.913  16.976  46.696  1.00  7.08           N
ANISOU 7865  N   SER B 213      674    925   1090    -11    -47    -55       N
ATOM   7867  CA  SER B 213      63.154  17.422  46.071  1.00  6.55           C
ANISOU 7867  CA  SER B 213      793    829    866    -92     66      4       C
ATOM   7869  CB  SER B 213      62.831  18.416  45.000  1.00  6.60           C
ANISOU 7869  CB  SER B 213      545   1032    927     11   -196     18       C
ATOM   7872  OG  SER B 213      64.004  18.999  44.434  1.00  9.48           O
ANISOU 7872  OG  SER B 213     1094   1226   1281   -117    432    256       O
ATOM   7874  C   SER B 213      63.971  18.198  47.116  1.00  7.04           C
ANISOU 7874  C   SER B 213      877   1011    787     23    -55    -22       C
ATOM   7875  O   SER B 213      63.527  19.266  47.564  1.00  8.08           O
ANISOU 7875  O   SER B 213     1033   1179    858    -38      4   -193       O
ATOM   7876  N   VAL B 214      65.176  17.725  47.420  1.00  7.32           N
ANISOU 7876  N   VAL B 214      907    960    914    -22     27    -86       N
ATOM   7878  CA  VAL B 214      66.065  18.412  48.332  1.00  8.50           C
ANISOU 7878  CA  VAL B 214      992   1117   1118     26    -31      7       C
ATOM   7880  CB  VAL B 214      66.662  17.473  49.325  1.00  9.49           C
ANISOU 7880  CB  VAL B 214     1135   1234   1236    -41    -99     20       C
ATOM   7882  CG1 VAL B 214      67.640  18.265  50.220  1.00  9.17           C
ANISOU 7882  CG1 VAL B 214     1216   1187   1081    158   -197     -2       C
ATOM   7886  CG2 VAL B 214      65.557  16.808  50.137  1.00 11.30           C
ANISOU 7886  CG2 VAL B 214     1389   1327   1576     58    -56    153       C
ATOM   7890  C   VAL B 214      67.181  18.986  47.493  1.00  8.26           C
ANISOU 7890  C   VAL B 214      916   1055   1164    -59    -44     -4       C
ATOM   7891  O   VAL B 214      67.989  18.241  46.905  1.00  9.17           O
ANISOU 7891  O   VAL B 214      800   1215   1469    -74    237    171       O
ATOM   7892  N   GLU B 215      67.172  20.293  47.357  1.00  8.23           N
ANISOU 7892  N   GLU B 215      917   1057   1150     26   -148    -24       N
ATOM   7894  CA  GLU B 215      68.211  20.975  46.602  1.00  9.54           C
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ANISOU 7894  CA  GLU B 215     1134   1246   1244      5      1     10       C
ATOM   7896  CB  GLU B 215      67.662  22.184  45.830  1.00 10.10           C
ANISOU 7896  CB  GLU B 215     1238   1336   1261   -114    -15     54       C
ATOM   7899  CG  GLU B 215      66.611  21.801  44.781  1.00 13.81           C
ANISOU 7899  CG  GLU B 215     1578   1910   1758   -121    -99     21       C
ATOM   7902  CD  GLU B 215      67.090  21.091  43.527  1.00 17.31           C
ANISOU 7902  CD  GLU B 215     2165   2407   2002    -22     15    -95       C
ATOM   7903  OE1 GLU B 215      68.286  21.016  43.241  1.00 18.35           O
ANISOU 7903  OE1 GLU B 215     2158   2601   2211   -189   -201   -105       O
ATOM   7904  OE2 GLU B 215      66.196  20.584  42.790  1.00 18.32           O
ANISOU 7904  OE2 GLU B 215     2329   2396   2235    -24   -109     123       O
ATOM   7905  C   GLU B 215      69.311  21.454  47.534  1.00 10.31           C
ANISOU 7905  C   GLU B 215     1285   1363   1268    -32     -7     35       C
ATOM   7906  O   GLU B 215      69.015  21.990  48.613  1.00 10.95           O
ANISOU 7906  O   GLU B 215     1164   1485   1511     -3     42   -262       O
ATOM   7907  N   ILE B 216      70.582  21.269  47.143  1.00  8.84           N
ANISOU 7907  N   ILE B 216     1186   1120   1050     17    136    -41       N
ATOM   7909  CA  ILE B 216      71.663  21.828  47.943  1.00  9.55           C
ANISOU 7909  CA  ILE B 216     1186   1120   1323    -38     53    154       C
ATOM   7911  CB  ILE B 216      73.019  21.179  47.676  1.00  9.77           C
ANISOU 7911  CB  ILE B 216     1333    987   1390   -102     84     95       C
ATOM   7913  CG1 ILE B 216      72.965  19.655  47.786  1.00 10.93           C
ANISOU 7913  CG1 ILE B 216     1542   1161   1448    140    -36     77       C
ATOM   7916  CD1 ILE B 216      72.520  19.201  49.103  1.00 12.05           C
ANISOU 7916  CD1 ILE B 216     1598   1323   1658     92    147     24       C
ATOM   7920  CG2 ILE B 216      74.070  21.754  48.722  1.00 13.23           C
ANISOU 7920  CG2 ILE B 216     1725   1640   1660     77    -40     68       C
ATOM   7924  C   ILE B 216      71.764  23.376  47.628  1.00  9.10           C
ANISOU 7924  C   ILE B 216     1022   1150   1284    -74     58     42       C
ATOM   7925  O   ILE B 216      71.927  23.788  46.438  1.00  8.37           O
ANISOU 7925  O   ILE B 216      843   1177   1158   -225   -132    135       O
ATOM   7926  N   MET B 217      71.750  24.157  48.702  1.00  7.68           N
ANISOU 7926  N   MET B 217      609   1083   1225    -68     47     -9       N
ATOM   7928  CA  MET B 217      72.067  25.557  48.649  1.00  8.58           C
ANISOU 7928  CA  MET B 217      947   1130   1180     11    -66     39       C
ATOM   7930  CB  MET B 217      71.215  26.316  49.614  1.00  9.01           C
ANISOU 7930  CB  MET B 217     1087   1149   1187    -42    -41    -31       C
ATOM   7933  CG  MET B 217      71.532  27.850  49.786  1.00 10.49           C
ANISOU 7933  CG  MET B 217     1444   1082   1457    -75    -43    172       C
ATOM   7936  SD  MET B 217      70.285  28.672  50.856  1.00 12.06           S
ANISOU 7936  SD  MET B 217     1553   1472   1554    196     -5    -92       S
ATOM   7937  CE  MET B 217      68.809  28.514  49.872  1.00 13.78           C
ANISOU 7937  CE  MET B 217     1799   1689   1747    -59    188    138       C
ATOM   7941  C   MET B 217      73.554  25.671  49.012  1.00  7.98           C
ANISOU 7941  C   MET B 217      960    984   1088     -4    -22    -25       C
ATOM   7942  O   MET B 217      73.983  25.471  50.156  1.00  9.87           O
ANISOU 7942  O   MET B 217     1136   1378   1233     46    -49     97       O
ATOM   7943  N   GLY B 218      74.336  26.021  48.037  1.00  6.93           N
ANISOU 7943  N   GLY B 218      706    873   1053     42      0    -36       N
ATOM   7945  CA  GLY B 218      75.763  25.985  48.251  1.00  7.75           C
ANISOU 7945  CA  GLY B 218      864   1131    947    -81    -97     87       C
ATOM   7948  C   GLY B 218      76.297  27.058  49.196  1.00  6.37           C
ANISOU 7948  C   GLY B 218      761    859    800    -65     36      0       C
ATOM   7949  O   GLY B 218      75.642  28.068  49.536  1.00  7.36           O
ANISOU 7949  O   GLY B 218      587   1263    945   -128    -52   -133       O
ATOM   7950  N   ARG B 219      77.558  26.840  49.549  1.00  6.20           N
ANISOU 7950  N   ARG B 219      806    840    710     72   -118     12       N
ATOM   7952  CA  ARG B 219      78.279  27.638  50.533  1.00  7.04           C
ANISOU 7952  CA  ARG B 219      886    882    907    -45     22    -10       C
ATOM   7954  CB  ARG B 219      79.628  26.957  50.844  1.00  7.14           C
ANISOU 7954  CB  ARG B 219      952    863    896     36    -60    -26       C
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ATOM   7957  CG  ARG B 219      80.628  26.960  49.706  1.00  8.87           C
ANISOU 7957  CG  ARG B 219    1149   1134   1086    -17    -70     26       C
ATOM   7960  CD  ARG B 219      81.710  25.866  49.818  1.00  7.79           C
ANISOU 7960  CD  ARG B 219     949   1126    882   -107    134     61       C
ATOM   7963  NE  ARG B 219      82.748  26.206  50.807  1.00  9.90           N
ANISOU 7963  NE  ARG B 219    1196   1491   1074     14    -52     47       N
ATOM   7965  CZ  ARG B 219      83.739  25.379  51.123  1.00 10.34           C
ANISOU 7965  CZ  ARG B 219    1423   1320   1182    -15   -102     72       C
ATOM   7966  NH1 ARG B 219      83.743  24.157  50.604  1.00 11.14           N
ANISOU 7966  NH1 ARG B 219    1526   1458   1247    103    102    -40       N
ATOM   7969  NH2 ARG B 219      84.683  25.734  52.002  1.00  7.84           N
ANISOU 7969  NH2 ARG B 219     996    873   1108     23    -20    124       N
ATOM   7972  C   ARG B 219      78.484  29.081  50.080  1.00  7.31           C
ANISOU 7972  C   ARG B 219     964    858    955     99    -33    -59       C
ATOM   7973  O   ARG B 219      78.874  29.954  50.862  1.00  7.45           O
ANISOU 7973  O   ARG B 219     779    964   1087     54     10   -205       O
ATOM   7974  N   GLY B 220      78.387  29.287  48.780  1.00  6.52           N
ANISOU 7974  N   GLY B 220     907    787    781     -8     25     42       N
ATOM   7976  CA  GLY B 220      78.409  30.629  48.260  1.00  8.26           C
ANISOU 7976  CA  GLY B 220    1232   1001    905     81    -41    -29       C
ATOM   7979  C   GLY B 220      77.242  31.516  48.666  1.00  7.37           C
ANISOU 7979  C   GLY B 220     929   1039    830     70   -106      3       C
ATOM   7980  O   GLY B 220      77.418  32.743  48.606  1.00  8.65           O
ANISOU 7980  O   GLY B 220    1099   1119   1068    340   -111     55       O
ATOM   7981  N   TYR B 221      76.114  30.929  49.092  1.00  7.64           N
ANISOU 7981  N   TYR B 221    1072   1041    787     37    -28    -12       N
ATOM   7983  CA  TYR B 221      74.967  31.663  49.586  1.00  7.64           C
ANISOU 7983  CA  TYR B 221    1014   1017    870     92   -155     90       C
ATOM   7985  CB  TYR B 221      73.672  30.854  49.426  1.00  7.23           C
ANISOU 7985  CB  TYR B 221     960    899    887     60    -74     86       C
ATOM   7988  CG  TYR B 221      73.155  30.704  47.991  1.00  7.13           C
ANISOU 7988  CG  TYR B 221     665   1180    863   -113     31     80       C
ATOM   7989  CD1 TYR B 221      73.196  29.500  47.340  1.00  8.62           C
ANISOU 7989  CD1 TYR B 221    1032   1177   1063    -86     88    261       C
ATOM   7991  CE1 TYR B 221      72.751  29.378  46.037  1.00 10.83           C
ANISOU 7991  CE1 TYR B 221    1308   1493   1311   -316   -130     55       C
ATOM   7993  CZ  TYR B 221      72.198  30.503  45.393  1.00 12.21           C
ANISOU 7993  CZ  TYR B 221    1491   1724   1423     79    -47    -42       C
ATOM   7994  OH  TYR B 221      71.696  30.425  44.065  1.00 14.19           O
ANISOU 7994  OH  TYR B 221    1301   2531   1557     51   -207    160       O
ATOM   7996  CE2 TYR B 221      72.128  31.685  46.046  1.00 10.38           C
ANISOU 7996  CE2 TYR B 221    1243   1385   1313   -184    -82    331       C
ATOM   7998  CD2 TYR B 221      72.588  31.791  47.329  1.00  9.62           C
ANISOU 7998  CD2 TYR B 221    1246   1172   1235   -163     63    -24       C
ATOM   8000  C   TYR B 221      75.110  31.869  51.094  1.00  8.55           C
ANISOU 8000  C   TYR B 221    1222   1053    971     35    -17    -38       C
ATOM   8001  O   TYR B 221      75.737  31.045  51.754  1.00  9.15           O
ANISOU 8001  O   TYR B 221    1659   1026    790    301   -188   -143       O
ATOM   8002  N   ALA B 222      74.590  32.977  51.612  1.00  8.75           N
ANISOU 8002  N   ALA B 222    1042   1052   1230    134     29    102       N
ATOM   8004  CA  ALA B 222      74.490  33.151  53.032  1.00  9.59           C
ANISOU 8004  CA  ALA B 222    1092   1207   1344     87     -1     51       C
ATOM   8006  CB  ALA B 222      74.801  34.548  53.454  1.00 11.40           C
ANISOU 8006  CB  ALA B 222    1295   1475   1559    -94    103    -38       C
ATOM   8010  C   ALA B 222      73.055  32.801  53.417  1.00 10.24           C
ANISOU 8010  C   ALA B 222    1158   1337   1395    -75     98    121       C
ATOM   8011  O   ALA B 222      72.111  33.257  52.772  1.00  8.71           O
ANISOU 8011  O   ALA B 222     748   1108   1453   -277    191    100       O
ATOM   8012  N   TRP B 223      72.927  31.966  54.433  1.00 10.57           N
ANISOU 8012  N   TRP B 223    1245   1424   1345     17     81     91       N
ATOM   8014  CA  TRP B 223      71.617  31.648  55.060  1.00  9.73           C
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ANISOU	8014	CA	TRP	B	223	1096	1348	1250	-25	-9	12		C
ATOM	8016	CB	TRP	B	223	71.184	30.192	54.891	1.00	10.75			C
ANISOU	8016	CB	TRP	B	223	1287	1554	1243	-72	26	34		C
ATOM	8019	CG	TRP	B	223	69.899	29.871	55.706	1.00	8.42			C
ANISOU	8019	CG	TRP	B	223	965	1209	1024	-108	-24	-124		C
ATOM	8020	CD1	TRP	B	223	68.777	30.564	55.722	1.00	11.01			C
ANISOU	8020	CD1	TRP	B	223	1576	1392	1216	-25	-62	78		C
ATOM	8022	NE1	TRP	B	223	67.868	30.014	56.604	1.00	10.77			N
ANISOU	8022	NE1	TRP	B	223	1066	1479	1544	-85	238	46		N
ATOM	8024	CE2	TRP	B	223	68.482	28.978	57.262	1.00	9.41			C
ANISOU	8024	CE2	TRP	B	223	1173	1284	1116	88	205	-33		C
ATOM	8025	CD2	TRP	B	223	69.753	28.847	56.705	1.00	10.61			C
ANISOU	8025	CD2	TRP	B	223	1055	1431	1545	-103	35	2		C
ATOM	8026	CE3	TRP	B	223	70.584	27.825	57.182	1.00	10.23			C
ANISOU	8026	CE3	TRP	B	223	1311	1107	1466	-59	-10	144		C
ATOM	8028	CZ3	TRP	B	223	70.117	26.979	58.160	1.00	9.84			C
ANISOU	8028	CZ3	TRP	B	223	1148	1407	1182	45	95	-61		C
ATOM	8034	C	TRP	B	223	71.869	31.908	56.530	1.00	12.21			C
ANISOU	8034	C	TRP	B	223	1507	1706	1426	23	106	131		C
ATOM	8035	O	TRP	B	223	72.679	31.207	57.206	1.00	12.56			O
ANISOU	8035	O	TRP	B	223	1512	1769	1490	191	130	164		O
ATOM	8036	N	LEU	B	224	71.202	32.910	57.044	1.00	13.37			N
ANISOU	8036	N	LEU	B	224	1845	1630	1605	125	-8	85		N
ATOM	8038	CA	LEU	B	224	71.365	33.268	58.431	1.00	16.15			C
ANISOU	8038	CA	LEU	B	224	2148	1939	2046	20	-24	-15		C
ATOM	8043	CG	LEU	B	224	73.181	34.812	57.629	1.00	16.95			C
ANISOU	8043	CG	LEU	B	224	2208	2006	2223	-30	-11	-31		C
ATOM	8045	CD1	LEU	B	224	73.511	36.294	57.545	1.00	17.91			C
ANISOU	8045	CD1	LEU	B	224	2639	2042	2123	-104	95	-78		C
ATOM	8049	CD2	LEU	B	224	74.332	33.994	58.192	1.00	16.82			C
ANISOU	8049	CD2	LEU	B	224	2057	2028	2304	-97	-33	-44		C
ATOM	8237	CG	PHE	B	238	76.258	39.198	55.928	1.00	11.60			C
ANISOU	8237	CG	PHE	B	238	1602	1349	1453	-201	86	1		C
ATOM	8238	CD1	PHE	B	238	77.325	38.359	55.898	1.00	14.20			C
ANISOU	8238	CD1	PHE	B	238	1878	1593	1923	-184	230	-20		C
ATOM	8240	CE1	PHE	B	238	77.563	37.545	54.819	1.00	17.85			C
ANISOU	8240	CE1	PHE	B	238	2698	2083	2001	-70	-2	-56		C
ATOM	8242	CZ	PHE	B	238	76.710	37.550	53.782	1.00	16.16			C
ANISOU	8242	CZ	PHE	B	238	2221	1879	2037	-76	-146	-94		C
ATOM	8244	CE2	PHE	B	238	75.662	38.347	53.774	1.00	14.44			C
ANISOU	8244	CE2	PHE	B	238	1901	1679	1905	-159	402	-28		C
ATOM	8246	CD2	PHE	B	238	75.406	39.189	54.909	1.00	15.83			C
ANISOU	8246	CD2	PHE	B	238	2434	1791	1786	-218	-94	11		C
ATOM	8287	CG2	THR	B	241	80.981	44.091	54.329	1.00	10.17			C
ANISOU	8287	CG2	THR	B	241	1011	1501	1352	101	-35	70		C
ATOM	8295	CA	LEU	B	242	77.280	44.645	51.519	1.00	9.28			C
ANISOU	8295	CA	LEU	B	242	1236	1175	1112	60	39	-11		C
ATOM	8297	CB	LEU	B	242	76.281	43.555	51.232	1.00	7.76			C
ANISOU	8297	CB	LEU	B	242	916	1129	902	-10	71	213		C
ATOM	8300	CG	LEU	B	242	76.869	42.164	51.479	1.00	12.76			C
ANISOU	8300	CG	LEU	B	242	1718	1540	1588	50	111	29		C
ATOM	8302	CD1	LEU	B	242	75.784	41.132	51.539	1.00	14.27			C
ANISOU	8302	CD1	LEU	B	242	1867	1780	1772	-47	10	-24		C
ATOM	8306	CD2	LEU	B	242	77.885	41.781	50.462	1.00	13.59			C
ANISOU	8306	CD2	LEU	B	242	1684	1512	1967	82	128	-47		C
ATOM	8348	CG	ARG	B	245	81.698	46.720	48.611	1.00	6.78			C
ANISOU	8348	CG	ARG	B	245	927	895	752	234	-169	38		C
ATOM	8354	NE	ARG	B	245	83.975	46.857	47.851	1.00	7.02			N
ANISOU	8354	NE	ARG	B	245	1161	656	848	260	-263	-45		N
ATOM	8360	NH2	ARG	B	245	85.939	46.653	46.748	1.00	12.77			N
ANISOU	8360	NH2	ARG	B	245	1821	1633	1397	-12	97	40		N

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ATOM   8372  CG  GLN B 246      77.461  45.847  46.729  1.00  6.40           C
ANISOU 8372  CG  GLN B 246     868     968     595     185     166     160    C
ATOM   8375  CD  GLN B 246      76.489  44.724  46.642  1.00  8.67           C
ANISOU 8375  CD  GLN B 246    1178    1137     976     146       4     182    C
ATOM   8377  NE2 GLN B 246      77.025  43.476  46.649  1.00  9.11           N
ANISOU 8377  NE2 GLN B 246    1491     991     979     135      86    -126    N
ATOM   9400  CB  PRO C  17      97.800  29.455  58.563  1.00 34.98           C
ANISOU 9400  CB  PRO C  17    4463    4437    4388      12     -22      14    C
ATOM   9403  CG  PRO C  17      96.330  28.941  58.580  1.00 35.79           C
ANISOU 9403  CG  PRO C  17    4519    4590    4487      -9     -19      -6    C
ATOM   9406  CD  PRO C  17      95.684  29.442  59.846  1.00 36.57           C
ANISOU 9406  CD  PRO C  17    4638    4662    4594     -27      -8       3    C
ATOM  13815  CD1 ILE D   6      98.652  34.855  44.755  1.00 11.24           C
ANISOU13815  CD1 ILE D   6     967    1715    1587     -99     147      55    C
ATOM  14147  C   PRO D  28      93.756  38.921  58.263  1.00 18.28           C
ANISOU14147  C   PRO D  28    2471    2236    2236     -11       0     -41    C
ATOM  14149  N   VAL D  29      92.958  38.211  57.453  1.00 15.26           N
ANISOU14149  N   VAL D  29    1989    1914    1894      81     -47     -39    N
ATOM  14151  CA  VAL D  29      91.550  38.532  57.299  1.00 14.49           C
ANISOU14151  CA  VAL D  29    1971    1829    1704       8     -22     -42    C
ATOM  14153  CB  VAL D  29      91.037  38.537  55.861  1.00 13.03           C
ANISOU14153  CB  VAL D  29    1637    1655    1657     -27    -148     -15    C
ATOM  14155  CG1 VAL D  29      89.523  38.782  55.855  1.00 15.29           C
ANISOU14155  CG1 VAL D  29    2005    1845    1958      44      49      47    C
ATOM  14159  CG2 VAL D  29      91.722  39.594  55.059  1.00 11.37           C
ANISOU14159  CG2 VAL D  29    1427    1560    1333     169    -206     -91    C
ATOM  14163  C   VAL D  29      90.873  37.481  58.152  1.00 13.14           C
ANISOU14163  C   VAL D  29    1697    1686    1608       8     -31     -12    C
ATOM  14164  O   VAL D  29      90.679  36.338  57.744  1.00 13.08           O
ANISOU14164  O   VAL D  29    1822    1770    1377     126    -128     160    O
ATOM  14165  N   TYR D  30      90.528  37.878  59.366  1.00 12.71           N
ANISOU14165  N   TYR D  30    1717    1629    1483     -42     -30      45    N
ATOM  14167  CA  TYR D  30      89.917  36.961  60.338  1.00 13.61           C
ANISOU14167  CA  TYR D  30    1794    1757    1620     -68       4       1    C
ATOM  14169  CB  TYR D  30      88.625  36.297  59.903  1.00 12.88           C
ANISOU14169  CB  TYR D  30    1773    1774    1344       2      26       0    C
ATOM  14172  CG  TYR D  30      87.996  35.415  60.974  1.00 12.15           C
ANISOU14172  CG  TYR D  30    1410    1641    1562     -33     -45     -48    C
ATOM  14173  CD1 TYR D  30      87.839  35.893  62.283  1.00 12.33           C
ANISOU14173  CD1 TYR D  30    1424    1787    1471      79     -16      -8    C
ATOM  14175  CE1 TYR D  30      87.224  35.133  63.263  1.00 11.25           C
ANISOU14175  CE1 TYR D  30    1378    1648    1248    -103    -270     180    C
ATOM  14177  CZ  TYR D  30      86.842  33.817  62.970  1.00 11.44           C
ANISOU14177  CZ  TYR D  30    1314    1558    1474      63    -186     -25    C
ATOM  14178  OH  TYR D  30      86.227  32.988  63.919  1.00 15.52           O
ANISOU14178  OH  TYR D  30    1962    2030    1906      98    -314     130    O
ATOM  14180  CE2 TYR D  30      87.024  33.334  61.713  1.00 10.95           C
ANISOU14180  CE2 TYR D  30    1467    1195    1496     -41     -88     -51    C
ATOM  14182  CD2 TYR D  30      87.633  34.108  60.729  1.00 10.27           C
ANISOU14182  CD2 TYR D  30    1319    1564    1018      18     -61     -85    C
ATOM  14184  C   TYR D  30      90.868  35.901  60.811  1.00 14.13           C
ANISOU14184  C   TYR D  30    1912    1734    1723     -96     -28      40    C
ATOM  14185  O   TYR D  30      91.460  36.112  61.832  1.00 16.09           O
ANISOU14185  O   TYR D  30    2347    1950    1817    -183     -19     -48    O
ATOM  14186  N   ASP D  31      91.051  34.790  60.096  1.00 13.59           N
ANISOU14186  N   ASP D  31    1877    1833    1451     -38      36     -64    N
ATOM  14188  CA  ASP D  31      91.725  33.605  60.642  1.00 13.48           C
ANISOU14188  CA  ASP D  31    1683    1815    1622     -90      -7     -27    C
ATOM  14190  CB  ASP D  31      90.711  32.435  60.909  1.00 14.66           C
ANISOU14190  CB  ASP D  31    1849    1985    1735    -136     -28     -99    C
ATOM  14193  CG  ASP D  31      89.882  32.053  59.695  1.00 14.55           C
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ANISOU14193  CG  ASP D  31     1815   1942   1769    -25    -22     10       C
ATOM  14194  OD1 ASP D  31      89.991  32.720  58.652  1.00 13.21           O
ANISOU14194  OD1 ASP D  31     1607   1940   1471     55     93    -73       O
ATOM  14195  OD2 ASP D  31      89.066  31.070  59.737  1.00 16.83           O
ANISOU14195  OD2 ASP D  31     2285   2146   1961   -184    -45   -108       O
ATOM  14196  C   ASP D  31      92.871  33.073  59.782  1.00 13.68           C
ANISOU14196  C   ASP D  31     1751   1737   1709    -12    -51    -63       C
ATOM  14197  O   ASP D  31      93.443  32.051  60.076  1.00 15.61           O
ANISOU14197  O   ASP D  31     1805   2084   2042    137   -154     41       O
ATOM  14198  N   LYS D  32      93.162  33.759  58.696  1.00 13.03           N
ANISOU14198  N   LYS D  32     1644   1753   1550     30     56      1       N
ATOM  14200  CA  LYS D  32      94.235  33.367  57.758  1.00 11.84           C
ANISOU14200  CA  LYS D  32     1344   1647   1506     12     -2     -4       C
ATOM  14202  CB  LYS D  32      93.787  32.322  56.750  1.00 11.86           C
ANISOU14202  CB  LYS D  32     1374   1623   1507    -11    196     24       C
ATOM  14205  CG  LYS D  32      92.673  32.731  55.856  1.00 12.00           C
ANISOU14205  CG  LYS D  32     1603   1565   1390    -64    -79    -16       C
ATOM  14208  CD  LYS D  32      91.951  31.532  55.143  1.00  9.83           C
ANISOU14208  CD  LYS D  32      908   1273   1552    252     42     41       C
ATOM  14211  CE  LYS D  32      90.911  30.958  55.993  1.00 10.88           C
ANISOU14211  CE  LYS D  32     1342   1343   1446     86     40     88       C
ATOM  14214  NZ  LYS D  32      89.731  31.898  56.048  1.00 10.04           N
ANISOU14214  NZ  LYS D  32     1383    796   1636    234    131   -253       N
ATOM  14218  C   LYS D  32      94.824  34.589  57.052  1.00 11.29           C
ANISOU14218  C   LYS D  32     1368   1572   1349     73      2     17       C
ATOM  14219  O   LYS D  32      94.199  35.626  56.881  1.00  9.87           O
ANISOU14219  O   LYS D  32     1278   1400   1070     96    128    -52       O
ATOM  14220  N   PRO D  33      96.059  34.444  56.580  1.00 11.10           N
ANISOU14220  N   PRO D  33     1270   1532   1413     36     48    101       N
ATOM  14221  CA  PRO D  33      96.752  35.556  55.934  1.00 11.36           C
ANISOU14221  CA  PRO D  33     1426   1388   1499     24     29     41       C
ATOM  14223  CB  PRO D  33      98.045  34.932  55.445  1.00 11.62           C
ANISOU14223  CB  PRO D  33     1358   1490   1566      0    -33     84       C
ATOM  14226  CG  PRO D  33      98.211  33.647  56.306  1.00 12.82           C
ANISOU14226  CG  PRO D  33     1335   1648   1887     82    191    237       C
ATOM  14229  CD  PRO D  33      96.807  33.186  56.534  1.00 12.41           C
ANISOU14229  CD  PRO D  33     1475   1627   1613    -31    135     88       C
ATOM  14232  C   PRO D  33      95.963  36.049  54.725  1.00 10.95           C
ANISOU14232  C   PRO D  33     1312   1372   1474     47    -36     75       C
ATOM  14233  O   PRO D  33      95.418  35.216  53.964  1.00 11.32           O
ANISOU14233  O   PRO D  33     1701   1121   1476     36     43    138       O
ATOM  14234  N   MET D  34      95.992  37.360  54.493  1.00 11.68           N
ANISOU14234  N   MET D  34     1444   1423   1572    -51    -34     43       N
ATOM  14236  CA  MET D  34      95.230  38.000  53.378  1.00 11.29           C
ANISOU14236  CA  MET D  34     1202   1496   1588    -19     22     97       C
ATOM  14238  CB  MET D  34      95.389  39.530  53.360  1.00 12.61           C
ANISOU14238  CB  MET D  34     1353   1658   1777    -34     31     53       C
ATOM  14241  CG  MET D  34      94.482  40.438  52.315  1.00 14.19           C
ANISOU14241  CG  MET D  34     1906   1784   1699    135    213     66       C
ATOM  14249  C   MET D  34      95.563  37.380  52.048  1.00 11.30           C
ANISOU14249  C   MET D  34     1245   1372   1675    -18     58     90       C
ATOM  14250  O   MET D  34      94.689  37.200  51.247  1.00  9.38           O
ANISOU14250  O   MET D  34     1217   1069   1276    174    121    396       O
ATOM  14251  N   ILE D  35      96.850  37.004  51.799  1.00 12.32           N
ANISOU14251  N   ILE D  35     1241   1669   1767    105     -9    109       N
ATOM  14253  CA  ILE D  35      97.193  36.467  50.504  1.00 12.29           C
ANISOU14253  CA  ILE D  35     1376   1601   1690     75     20     76       C
ATOM  14255  CB  ILE D  35      98.770  36.389  50.341  1.00 13.91           C
ANISOU14255  CB  ILE D  35     1567   1797   1920     98    -33     17       C
ATOM  14257  CG1 ILE D  35      99.101  36.238  48.856  1.00 14.65           C
ANISOU14257  CG1 ILE D  35     1693   1906   1964     70     88     -1       C
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ATOM  14264  CG2 ILE D  35      99.307  35.288  51.176  1.00 15.92           C
ANISOU14264  CG2 ILE D  35    1905   2109   2034     68      1     49       C
ATOM  14268  C   ILE D  35      96.498  35.168  50.153  1.00 11.67           C
ANISOU14268  C   ILE D  35    1281   1606   1544    130    -14     99       C
ATOM  14269  O   ILE D  35      96.377  34.790  48.972  1.00 10.70           O
ANISOU14269  O   ILE D  35    1306   1447   1312     96     34    167       O
ATOM  14270  N   TYR D  36      96.056  34.419  51.155  1.00 10.53           N
ANISOU14270  N   TYR D  36    1161   1437   1403     60      5     89       N
ATOM  14272  CA  TYR D  36      95.335  33.188  50.852  1.00 11.54           C
ANISOU14272  CA  TYR D  36    1412   1519   1453     56    -25     78       C
ATOM  14274  CB  TYR D  36      94.888  32.521  52.171  1.00 11.49           C
ANISOU14274  CB  TYR D  36    1406   1593   1366    -43    -74     89       C
ATOM  14277  CG  TYR D  36      95.908  31.654  52.876  1.00 12.21           C
ANISOU14277  CG  TYR D  36    1504   1569   1566     51     63    120       C
ATOM  14278  CD1 TYR D  36      97.247  31.865  52.716  1.00 12.64           C
ANISOU14278  CD1 TYR D  36    1451   1692   1659     70    -75     76       C
ATOM  14280  CE1 TYR D  36      98.190  31.099  53.386  1.00 13.00           C
ANISOU14280  CE1 TYR D  36    1479   1670   1790     91    -17    175       C
ATOM  14282  CZ  TYR D  36      97.782  30.131  54.245  1.00 13.08           C
ANISOU14282  CZ  TYR D  36    1378   1705   1885    -11     23    104       C
ATOM  14283  OH  TYR D  36      98.695  29.367  54.891  1.00 12.45           O
ANISOU14283  OH  TYR D  36    1423   1994   1314   -109    109    304       O
ATOM  14285  CE2 TYR D  36      96.417  29.877  54.435  1.00 12.76           C
ANISOU14285  CE2 TYR D  36    1334   1814   1697    -23     42    138       C
ATOM  14287  CD2 TYR D  36      95.489  30.661  53.753  1.00 13.60           C
ANISOU14287  CD2 TYR D  36    1973   1556   1637     74    -52     47       C
ATOM  14289  C   TYR D  36      94.043  33.425  49.992  1.00  9.82           C
ANISOU14289  C   TYR D  36    1073   1374   1282      0     88     88       C
ATOM  14290  O   TYR D  36      93.612  32.557  49.234  1.00  9.73           O
ANISOU14290  O   TYR D  36    1007   1517   1172    349     55     73       O
ATOM  14291  N   TYR D  37      93.488  34.634  50.087  1.00 10.75           N
ANISOU14291  N   TYR D  37    1263   1477   1342    -21    112     39       N
ATOM  14293  CA  TYR D  37      92.214  34.958  49.455  1.00 10.89           C
ANISOU14293  CA  TYR D  37    1362   1395   1379     48     47     65       C
ATOM  14295  CB  TYR D  37      91.522  36.136  50.133  1.00 11.33           C
ANISOU14295  CB  TYR D  37    1499   1499   1306      2     19      5       C
ATOM  14298  CG  TYR D  37      91.108  35.805  51.562  1.00  9.88           C
ANISOU14298  CG  TYR D  37    1326   1195   1230     25     52     28       C
ATOM  14299  CD1 TYR D  37      91.979  35.991  52.618  1.00  9.15           C
ANISOU14299  CD1 TYR D  37     963   1372   1141    -54    108     20       C
ATOM  14301  CE1 TYR D  37      91.598  35.659  53.937  1.00  7.73           C
ANISOU14301  CE1 TYR D  37     762   1146   1028     24     55    -40       C
ATOM  14303  CZ  TYR D  37      90.377  35.137  54.177  1.00  9.03           C
ANISOU14303  CZ  TYR D  37    1233   1163   1033   -129    -10    -79       C
ATOM  14304  OH  TYR D  37      90.044  34.798  55.489  1.00  7.85           O
ANISOU14304  OH  TYR D  37    1242    879    860   -229   -210    103       O
ATOM  14306  CE2 TYR D  37      89.471  34.933  53.125  1.00  9.02           C
ANISOU14306  CE2 TYR D  37     996   1165   1265    144    -68     56       C
ATOM  14308  CD2 TYR D  37      89.838  35.259  51.845  1.00  9.07           C
ANISOU14308  CD2 TYR D  37    1152   1144   1148    120   -118    -10       C
ATOM  14310  C   TYR D  37      92.421  35.100  47.961  1.00 10.54           C
ANISOU14310  C   TYR D  37    1242   1428   1334    132     90     92       C
ATOM  14311  O   TYR D  37      91.931  34.316  47.193  1.00 10.33           O
ANISOU14311  O   TYR D  37     924   1491   1508    125    200    156       O
ATOM  14312  N   PRO D  38      93.240  36.017  47.532  1.00 11.44           N
ANISOU14312  N   PRO D  38    1441   1449   1454    149     39     38       N
ATOM  14313  CA  PRO D  38      93.554  36.040  46.089  1.00 11.86           C
ANISOU14313  CA  PRO D  38    1554   1535   1417     17     61     74       C
ATOM  14315  CB  PRO D  38      94.448  37.255  45.967  1.00 12.13           C
ANISOU14315  CB  PRO D  38    1448   1589   1570     26      5      6       C
ATOM  14318  CG  PRO D  38      94.935  37.510  47.318  1.00 13.55           C
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ANISOU14318	CG	PRO	D	38	1789	1690	1669	73	79	62		C
ATOM 14321	CD	PRO	D	38	93.852	37.147	48.241	1.00	12.23			C
ANISOU14321	CD	PRO	D	38	1475	1696	1475	76	32	93		C
ATOM 14324	C	PRO	D	38	94.220	34.753	45.543	1.00	10.91			C
ANISOU14324	C	PRO	D	38	1358	1477	1310	-24	73	86		C
ATOM 14325	O	PRO	D	38	94.004	34.350	44.388	1.00	10.09			O
ANISOU14325	O	PRO	D	38	1382	1300	1151	-256	138	256		O
ATOM 14326	N	LEU	D	39	95.026	34.089	46.352	1.00	11.37			N
ANISOU14326	N	LEU	D	39	1533	1489	1297	-39	119	98		N
ATOM 14328	CA	LEU	D	39	95.603	32.814	45.930	1.00	11.05			C
ANISOU14328	CA	LEU	D	39	1456	1499	1241	-19	122	114		C
ATOM 14330	CB	LEU	D	39	96.607	32.295	46.964	1.00	11.17			C
ANISOU14330	CB	LEU	D	39	1423	1450	1371	32	114	-6		C
ATOM 14333	CG	LEU	D	39	97.095	30.880	46.629	1.00	12.36			C
ANISOU14333	CG	LEU	D	39	1555	1521	1617	67	51	24		C
ATOM 14335	CD1	LEU	D	39	97.993	30.865	45.380	1.00	15.12			C
ANISOU14335	CD1	LEU	D	39	1956	1943	1843	133	126	23		C
ATOM 14339	CD2	LEU	D	39	97.844	30.371	47.797	1.00	12.75			C
ANISOU14339	CD2	LEU	D	39	1810	1521	1512	285	82	-106		C
ATOM 14343	C	LEU	D	39	94.481	31.790	45.614	1.00	11.37			C
ANISOU14343	C	LEU	D	39	1542	1466	1312	-37	101	138		C
ATOM 14344	O	LEU	D	39	94.504	31.112	44.567	1.00	11.62			O
ANISOU14344	O	LEU	D	39	1642	1586	1187	-194	360	337		O
ATOM 14345	N	SER	D	40	93.478	31.691	46.510	1.00	10.55			N
ANISOU14345	N	SER	D	40	1326	1462	1218	36	18	83		N
ATOM 14347	CA	SER	D	40	92.364	30.785	46.311	1.00	11.33			C
ANISOU14347	CA	SER	D	40	1398	1496	1410	35	60	114		C
ATOM 14349	CB	SER	D	40	91.389	30.798	47.524	1.00	11.65			C
ANISOU14349	CB	SER	D	40	1377	1674	1373	-4	54	59		C
ATOM 14352	OG	SER	D	40	90.555	31.978	47.533	1.00	12.46			O
ANISOU14352	OG	SER	D	40	1482	1854	1398	-110	470	-84		O
ATOM 14354	C	SER	D	40	91.594	31.122	45.045	1.00	10.33			C
ANISOU14354	C	SER	D	40	1080	1485	1360	69	39	35		C
ATOM 14355	O	SER	D	40	91.125	30.217	44.332	1.00	10.96			O
ANISOU14355	O	SER	D	40	682	1795	1684	240	12	136		O
ATOM 14356	N	THR	D	41	91.524	32.416	44.741	1.00	9.61			N
ANISOU14356	N	THR	D	41	926	1362	1363	37	18	88		N
ATOM 14358	CA	THR	D	41	90.828	32.822	43.548	1.00	10.81			C
ANISOU14358	CA	THR	D	41	1326	1400	1379	-59	35	55		C
ATOM 14360	CB	THR	D	41	90.734	34.359	43.467	1.00	11.27			C
ANISOU14360	CB	THR	D	41	1353	1494	1434	87	-6	-6		C
ATOM 14362	OG1	THR	D	41	89.828	34.828	44.474	1.00	12.66			O
ANISOU14362	OG1	THR	D	41	1444	1901	1462	121	124	-92		O
ATOM 14364	CG2	THR	D	41	90.174	34.798	42.119	1.00	10.27			C
ANISOU14364	CG2	THR	D	41	1238	1188	1475	-31	-138	-148		C
ATOM 14368	C	THR	D	41	91.490	32.248	42.286	1.00	11.57			C
ANISOU14368	C	THR	D	41	1481	1484	1432	-11	-28	7		C
ATOM 14369	O	THR	D	41	90.798	31.707	41.413	1.00	11.54			O
ANISOU14369	O	THR	D	41	1323	1689	1373	-208	-200	120		O
ATOM 14370	N	LEU	D	42	92.804	32.380	42.179	1.00	10.14			N
ANISOU14370	N	LEU	D	42	1296	1329	1225	-81	-38	93		N
ATOM 14372	CA	LEU	D	42	93.507	31.756	41.077	1.00	11.90			C
ANISOU14372	CA	LEU	D	42	1534	1517	1467	-3	6	21		C
ATOM 14374	CB	LEU	D	42	94.961	32.086	41.121	1.00	12.05			C
ANISOU14374	CB	LEU	D	42	1580	1601	1397	-103	54	-37		C
ATOM 14377	CG	LEU	D	42	95.224	33.574	40.884	1.00	14.25			C
ANISOU14377	CG	LEU	D	42	1949	1667	1797	41	-125	-38		C
ATOM 14379	CD1	LEU	D	42	96.731	33.752	40.860	1.00	14.05			C
ANISOU14379	CD1	LEU	D	42	1853	1795	1687	-31	59	-31		C
ATOM 14383	CD2	LEU	D	42	94.647	34.164	39.610	1.00	14.01			C
ANISOU14383	CD2	LEU	D	42	1785	1827	1709	88	-41	-58		C

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ATOM  14387  C   LEU D  42      93.348  30.238  41.042  1.00 11.79           C
ANISOU14387  C   LEU D  42    1437   1539   1503     25    113     -1       C
ATOM  14388  O   LEU D  42      93.024  29.683  40.011  1.00 12.62           O
ANISOU14388  O   LEU D  42    1540   1629   1626     35    157    -28       O
ATOM  14389  N   MET D  43      93.463  29.592  42.186  1.00 12.35           N
ANISOU14389  N   MET D  43    1401   1569   1720    124     -7     14       N
ATOM  14391  CA  MET D  43      93.224  28.151  42.264  1.00 11.81           C
ANISOU14391  CA  MET D  43    1436   1489   1562     31     15    -38       C
ATOM  14393  CB  MET D  43      93.398  27.702  43.702  1.00 12.98           C
ANISOU14393  CB  MET D  43    1572   1591   1768     99    -69    -39       C
ATOM  14396  CG  MET D  43      94.863  27.795  44.195  1.00 12.17           C
ANISOU14396  CG  MET D  43    1384   1467   1773     88     21   -126       C
ATOM  14399  SD  MET D  43      95.078  27.432  45.997  1.00 12.56           S
ANISOU14399  SD  MET D  43    1500   1546   1723    325    323   -100       S
ATOM  14400  CE  MET D  43      94.788  25.680  45.995  1.00 14.32           C
ANISOU14400  CE  MET D  43    1713   1921   1805    -49     71    -58       C
ATOM  14404  C   MET D  43      91.821  27.756  41.754  1.00 12.65           C
ANISOU14404  C   MET D  43    1624   1594   1588      0      0    -44       C
ATOM  14405  O   MET D  43      91.681  26.776  40.996  1.00 11.64           O
ANISOU14405  O   MET D  43    1463   1536   1421     12    -89   -127       O
ATOM  14406  N   LEU D  44      90.792  28.483  42.174  1.00 12.15           N
ANISOU14406  N   LEU D  44    1504   1519   1591     27     31     24       N
ATOM  14408  CA  LEU D  44      89.438  28.181  41.725  1.00 14.17           C
ANISOU14408  CA  LEU D  44    1786   1810   1787     47    -29    -15       C
ATOM  14410  CB  LEU D  44      88.398  28.938  42.557  1.00 14.07           C
ANISOU14410  CB  LEU D  44    1803   1727   1813     80     14    -92       C
ATOM  14413  CG  LEU D  44      88.320  28.494  44.013  1.00 15.62           C
ANISOU14413  CG  LEU D  44    1956   1933   2045    104    -48      3       C
ATOM  14415  CD1 LEU D  44      87.620  29.556  44.902  1.00 19.16           C
ANISOU14415  CD1 LEU D  44    2471   2397   2410     59    105     10       C
ATOM  14419  CD2 LEU D  44      87.616  27.172  44.105  1.00 16.73           C
ANISOU14419  CD2 LEU D  44    1810   2280   2266    -21     -2    139       C
ATOM  14423  C   LEU D  44      89.221  28.401  40.253  1.00 14.05           C
ANISOU14423  C   LEU D  44    1760   1841   1736    -36     13    -63       C
ATOM  14424  O   LEU D  44      88.272  27.842  39.660  1.00 15.74           O
ANISOU14424  O   LEU D  44    1838   2231   1909   -111     38    -70       O
ATOM  14425  N   ALA D  45      90.052  29.238  39.666  1.00 13.84           N
ANISOU14425  N   ALA D  45    1652   1888   1717     15    -51   -135       N
ATOM  14427  CA  ALA D  45      90.095  29.436  38.231  1.00 13.52           C
ANISOU14427  CA  ALA D  45    1645   1800   1690    -26    -33    -33       C
ATOM  14429  CB  ALA D  45      90.722  30.723  37.905  1.00 13.79           C
ANISOU14429  CB  ALA D  45    1764   1808   1667     21    -25    -85       C
ATOM  14433  C   ALA D  45      90.829  28.290  37.529  1.00 13.47           C
ANISOU14433  C   ALA D  45    1567   1854   1696    -25     -6    -27       C
ATOM  14434  O   ALA D  45      90.907  28.281  36.303  1.00 13.33           O
ANISOU14434  O   ALA D  45    1442   2011   1611    -57    156   -126       O
ATOM  14435  N   GLY D  46      91.348  27.324  38.283  1.00 13.27           N
ANISOU14435  N   GLY D  46    1613   1769   1660    -41     26    -30       N
ATOM  14437  CA  GLY D  46      92.076  26.209  37.686  1.00 14.31           C
ANISOU14437  CA  GLY D  46    1714   1818   1903    -14    -58      0       C
ATOM  14440  C   GLY D  46      93.567  26.464  37.423  1.00 14.09           C
ANISOU14440  C   GLY D  46    1757   1797   1799     14     18     28       C
ATOM  14441  O   GLY D  46      94.202  25.684  36.735  1.00 14.78           O
ANISOU14441  O   GLY D  46    1912   1843   1861    -34    -51    -38       O
ATOM  14442  N   ILE D  47      94.121  27.532  37.986  1.00 13.28           N
ANISOU14442  N   ILE D  47    1643   1715   1686    -34    -31     -3       N
ATOM  14444  CA  ILE D  47      95.511  27.931  37.756  1.00 12.54           C
ANISOU14444  CA  ILE D  47    1570   1679   1515     50    -18     18       C
ATOM  14446  CB  ILE D  47      95.581  29.455  37.672  1.00 11.95           C
ANISOU14446  CB  ILE D  47    1504   1666   1367    -31    -39      4       C
ATOM  14448  CG1 ILE D  47      94.725  29.937  36.494  1.00 12.13           C
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ANISOU14448  CG1 ILE D  47     1416   1645   1547     60    -35     42       C
ATOM  14451  CD1 ILE D  47      94.571  31.426  36.407  1.00 11.78           C
ANISOU14451  CD1 ILE D  47     1567   1547   1360   -185     14     32       C
ATOM  14459  C   ILE D  47      96.357  27.397  38.887  1.00 13.58           C
ANISOU14459  C   ILE D  47     1697   1801   1662    -20    -25      8       C
ATOM  14460  O   ILE D  47      96.023  27.593  40.045  1.00 14.57           O
ANISOU14460  O   ILE D  47     1697   2032   1806     53   -119    -22       O
ATOM  14461  N   ARG D  48      97.367  26.627  38.517  1.00 13.04           N
ANISOU14461  N   ARG D  48     1568   1704   1680     -8     -7     55       N
ATOM  14463  CA  ARG D  48      98.299  26.013  39.431  1.00 13.81           C
ANISOU14463  CA  ARG D  48     1701   1811   1732     -3     -8     40       C
ATOM  14468  CG  ARG D  48      97.138  23.736  39.228  1.00 17.74           C
ANISOU14468  CG  ARG D  48     2293   2205   2240    -49      3     70       C
ATOM  14471  CD  ARG D  48      97.310  22.245  38.784  1.00 19.98           C
ANISOU14471  CD  ARG D  48     2757   2326   2507      0    -81     18       C
ATOM  14474  NE  ARG D  48      98.097  21.449  39.741  1.00 20.52           N
ANISOU14474  NE  ARG D  48     2777   2439   2580     31    -67     74       N
ATOM  14509  CD1 ILE D  50      98.520  30.073  41.872  1.00 11.36           C
ANISOU14509  CD1 ILE D  50     1361   1303   1651   -109     -9     83       C
ATOM  14782  CD2 LEU D  66     101.155  30.828  50.804  1.00 15.18           C
ANISOU14782  CD2 LEU D  66     1649   1917   2200    207    143    -33       C
ATOM  14837  C   ASN D  71     101.168  20.975  48.977  1.00 17.90           C
ANISOU14837  C   ASN D  71     2274   2289   2238      5     54     -8       C
ATOM  14838  O   ASN D  71     100.316  20.126  49.362  1.00 18.28           O
ANISOU14838  O   ASN D  71     2384   2273   2286    -68     -6    -71       O
ATOM  14839  N   TRP D  72     100.854  22.044  48.244  1.00 17.26           N
ANISOU14839  N   TRP D  72     2187   2201   2167    -72    119      4       N
ATOM  14841  CA  TRP D  72      99.504  22.295  47.805  1.00 16.86           C
ANISOU14841  CA  TRP D  72     2191   2137   2075    -28     51      3       C
ATOM  14843  CB  TRP D  72      99.123  23.750  48.040  1.00 16.48           C
ANISOU14843  CB  TRP D  72     2112   2156   1994     -2     73    -47       C
ATOM  14846  CG  TRP D  72      99.190  24.124  49.488  1.00 15.13           C
ANISOU14846  CG  TRP D  72     1898   1927   1923    -78    -34      6       C
ATOM  14847  CD1 TRP D  72      99.278  23.276  50.546  1.00 13.84           C
ANISOU14847  CD1 TRP D  72     1668   1875   1715    -79     44    -53       C
ATOM  14849  NE1 TRP D  72      99.312  23.986  51.718  1.00 12.36           N
ANISOU14849  NE1 TRP D  72     1437   1669   1590    -53    -63      7       N
ATOM  14851  CE2 TRP D  72      99.270  25.319  51.425  1.00 11.87           C
ANISOU14851  CE2 TRP D  72     1335   1574   1599    111     66     32       C
ATOM  14852  CD2 TRP D  72      99.194  25.434  50.023  1.00 12.19           C
ANISOU14852  CD2 TRP D  72     1244   1680   1705    167     33     13       C
ATOM  14853  CE3 TRP D  72      99.164  26.706  49.460  1.00 14.25           C
ANISOU14853  CE3 TRP D  72     1868   1793   1751    -21     -3    107       C
ATOM  14855  CZ3 TRP D  72      99.171  27.815  50.306  1.00 14.45           C
ANISOU14855  CZ3 TRP D  72     1879   1878   1731    -65    -38    -14       C
ATOM  14857  CH2 TRP D  72      99.273  27.661  51.704  1.00 13.79           C
ANISOU14857  CH2 TRP D  72     1765   1779   1696     32     -7     17       C
ATOM  14859  CZ2 TRP D  72      99.320  26.421  52.275  1.00 13.61           C
ANISOU14859  CZ2 TRP D  72     1711   1703   1755   -129     46      5       C
ATOM  14861  C   TRP D  72      99.238  21.939  46.351  1.00 17.41           C
ANISOU14861  C   TRP D  72     2242   2207   2166      0     24    -36       C
ATOM  14862  O   TRP D  72      98.186  22.278  45.837  1.00 17.58           O
ANISOU14862  O   TRP D  72     2172   2428   2080    -86     89    -64       O
ATOM  14863  N   GLY D  73     100.152  21.220  45.705  1.00 16.90           N
ANISOU14863  N   GLY D  73     2155   2192   2074    -91    103    -27       N
ATOM  14865  CA  GLY D  73      99.942  20.873  44.309  1.00 17.18           C
ANISOU14865  CA  GLY D  73     2236   2094   2195   -106     -9     40       C
ATOM  14868  C   GLY D  73     100.141  22.053  43.357  1.00 16.47           C
ANISOU14868  C   GLY D  73     2163   2035   2059    -68    -61     68       C
ATOM  14869  O   GLY D  73      99.595  22.045  42.261  1.00 17.24           O
ANISOU14869  O   GLY D  73     2312   2056   2182   -182    -95    102       O
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ATOM  14874  CB  LEU D  74     100.612  25.492  43.754  1.00 12.75           C
ANISOU14874  CB  LEU D  74    1568   1533   1742     59     34     30       C
ATOM  14877  CG  LEU D  74      99.200  25.509  44.303  1.00 13.84           C
ANISOU14877  CG  LEU D  74    1752   1700   1807    -44      1     28       C
ATOM  14879  CD1 LEU D  74      99.057  26.722  45.201  1.00 14.22           C
ANISOU14879  CD1 LEU D  74    1768   1807   1824    -68    137    -30       C
ATOM  14883  CD2 LEU D  74      98.146  25.513  43.166  1.00 12.74           C
ANISOU14883  CD2 LEU D  74    1677   1556   1607     36     51    103       C
ATOM  15339  CA  VAL D 106      94.699  39.207  40.751  1.00 11.00           C
ANISOU15339  CA  VAL D 106    1351   1469   1360     -6     -8     -2       C
ATOM  15341  CB  VAL D 106      94.095  37.993  41.406  1.00 10.26           C
ANISOU15341  CB  VAL D 106    1315   1292   1292     12    -21    -25       C
ATOM  15343  CG1 VAL D 106      95.174  37.204  42.185  1.00 10.61           C
ANISOU15343  CG1 VAL D 106    1560   1406   1061    162     34   -163       C
ATOM  15347  CG2 VAL D 106      93.033  38.385  42.322  1.00 11.05           C
ANISOU15347  CG2 VAL D 106    1341   1447   1407    163    -91    -18       C
ATOM  15371  O   LEU D 107      94.438  40.815  45.072  1.00 12.14           O
ANISOU15371  O   LEU D 107    1799   1652   1159   -146    -80     79       O
ATOM  15378  O   GLY D 108      95.611  40.743  48.665  1.00 15.45           O
ANISOU15378  O   GLY D 108    2006   1748   2117   -151     46    118       O
ATOM  15389  C   ASP D 109      92.737  42.993  48.209  1.00 14.09           C
ANISOU15389  C   ASP D 109    1805   1842   1706     27     -4     -8       C
ATOM  15390  O   ASP D 109      91.856  43.593  48.833  1.00 16.25           O
ANISOU15390  O   ASP D 109    2182   2346   1644    128     16   -193       O
ATOM  15391  N   ASN D 110      92.489  42.247  47.124  1.00 12.84           N
ANISOU15391  N   ASN D 110    1679   1629   1569    -49     38    -18       N
ATOM  15393  CA  ASN D 110      91.113  41.982  46.647  1.00 12.22           C
ANISOU15393  CA  ASN D 110    1509   1604   1528     48     28     40       C
ATOM  15395  CB  ASN D 110      91.063  41.988  45.147  1.00 12.92           C
ANISOU15395  CB  ASN D 110    1600   1685   1620    -54     59    -95       C
ATOM  15398  CG  ASN D 110      90.983  43.393  44.533  1.00 13.15           C
ANISOU15398  CG  ASN D 110    1680   1859   1457   -106     47    152       C
ATOM  15399  OD1 ASN D 110      90.241  43.561  43.564  1.00 15.33           O
ANISOU15399  OD1 ASN D 110    1450   2680   1693     35     87     50       O
ATOM  15400  ND2 ASN D 110      91.784  44.388  45.034  1.00  9.69           N
ANISOU15400  ND2 ASN D 110    1297   1664    720     79    -20    252       N
ATOM  15403  C   ASN D 110      90.552  40.630  47.130  1.00 12.08           C
ANISOU15403  C   ASN D 110    1454   1587   1547    -17     44    -18       C
ATOM  15404  O   ASN D 110      91.189  39.602  46.986  1.00 11.77           O
ANISOU15404  O   ASN D 110    1245   1667   1559   -140    115    168       O
ATOM  15405  N   LEU D 111      89.368  40.639  47.737  1.00 11.50           N
ANISOU15405  N   LEU D 111    1242   1524   1603     54    -41     47       N
ATOM  15407  CA  LEU D 111      88.732  39.439  48.250  1.00 11.92           C
ANISOU15407  CA  LEU D 111    1406   1594   1528     57    -62    -38       C
ATOM  15409  CB  LEU D 111      88.543  39.623  49.744  1.00 11.97           C
ANISOU15409  CB  LEU D 111    1338   1651   1559    -57    -63    -51       C
ATOM  15412  CG  LEU D 111      88.240  38.385  50.519  1.00 15.46           C
ANISOU15412  CG  LEU D 111    2063   1984   1827     20   -100     38       C
ATOM  15414  CD1 LEU D 111      88.606  38.587  51.977  1.00 17.03           C
ANISOU15414  CD1 LEU D 111    2399   2101   1971   -111    -42    -82       C
ATOM  15418  CD2 LEU D 111      86.734  38.168  50.378  1.00 17.60           C
ANISOU15418  CD2 LEU D 111    2212   2533   1941   -195     95    104       C
ATOM  15422  C   LEU D 111      87.353  39.248  47.569  1.00 11.55           C
ANISOU15422  C   LEU D 111    1369   1571   1447    -16    -15    -62       C
ATOM  15423  O   LEU D 111      86.504  40.145  47.658  1.00 12.57           O
ANISOU15423  O   LEU D 111    1554   1670   1549     16   -209   -107       O
ATOM  15424  N   TYR D 112      87.175  38.128  46.882  1.00  9.99           N
ANISOU15424  N   TYR D 112    1200   1303   1289    -50     48     53       N
ATOM  15426  CA  TYR D 112      85.934  37.814  46.198  1.00 11.39           C
ANISOU15426  CA  TYR D 112    1469   1432   1424    -27    -21     26       C
ATOM  15428  CB  TYR D 112      86.201  37.324  44.760  1.00 10.85           C
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ANISOU15428  CB  TYR D 112     1340   1469   1310     27     10     58      C
ATOM  15431  CG  TYR D 112      86.860  38.370  43.881  1.00 12.72          C
ANISOU15431  CG  TYR D 112     1518   1642   1671    -61    -13     62      C
ATOM  15432  CD1 TYR D 112      88.267  38.535  43.845  1.00 11.45          C
ANISOU15432  CD1 TYR D 112     1223   1641   1486   -158    -30     -1      C
ATOM  15434  CE1 TYR D 112      88.836  39.528  43.071  1.00 12.33          C
ANISOU15434  CE1 TYR D 112     1455   1912   1318    128     21     37      C
ATOM  15436  CZ  TYR D 112      88.059  40.297  42.237  1.00 14.31          C
ANISOU15436  CZ  TYR D 112     1649   1786   2002    132     81    191      C
ATOM  15437  OH  TYR D 112      88.635  41.269  41.435  1.00 11.73          O
ANISOU15437  OH  TYR D 112     1294   1571   1590    -39    223    -33      O
ATOM  15439  CE2 TYR D 112      86.695  40.102  42.207  1.00 13.93          C
ANISOU15439  CE2 TYR D 112     1697   1656   1937     16     -9     90      C
ATOM  15441  CD2 TYR D 112      86.108  39.144  43.034  1.00 13.84          C
ANISOU15441  CD2 TYR D 112     1398   1995   1865     19      9    141      C
ATOM  15443  C   TYR D 112      85.232  36.671  46.923  1.00 11.25          C
ANISOU15443  C   TYR D 112     1326   1509   1440    -68     26     96      C
ATOM  15444  O   TYR D 112      85.893  35.760  47.431  1.00  9.95          O
ANISOU15444  O   TYR D 112     1104   1465   1210   -232   -110    207      O
ATOM  15445  N   TYR D 113      83.905  36.660  46.864  1.00 11.44          N
ANISOU15445  N   TYR D 113     1439   1465   1441     55   -123     43      N
ATOM  15447  CA  TYR D 113      83.136  35.565  47.420  1.00 10.77          C
ANISOU15447  CA  TYR D 113     1166   1525   1399    -23    -64     38      C
ATOM  15449  CB  TYR D 113      83.074  35.645  48.934  1.00 11.10          C
ANISOU15449  CB  TYR D 113     1223   1471   1521    -58     -4    -27      C
ATOM  15452  CG  TYR D 113      82.595  34.322  49.535  1.00 10.43          C
ANISOU15452  CG  TYR D 113     1313   1169   1479   -120    -79   -109      C
ATOM  15453  CD1 TYR D 113      83.468  33.317  49.753  1.00  9.29          C
ANISOU15453  CD1 TYR D 113     1131   1227   1170    -75    -71     95      C
ATOM  15455  CE1 TYR D 113      83.048  32.051  50.219  1.00 10.49          C
ANISOU15455  CE1 TYR D 113     1289   1333   1364    -89   -263    220      C
ATOM  15457  CZ  TYR D 113      81.721  31.851  50.533  1.00 11.89          C
ANISOU15457  CZ  TYR D 113     1560   1584   1373      2     48    128      C
ATOM  15458  OH  TYR D 113      81.374  30.595  50.988  1.00 13.39          O
ANISOU15458  OH  TYR D 113     1555   1869   1661   -244    134    -14      O
ATOM  15460  CE2 TYR D 113      80.824  32.882  50.318  1.00 10.41          C
ANISOU15460  CE2 TYR D 113     1452   1232   1270   -138      9   -109      C
ATOM  15462  CD2 TYR D 113      81.297  34.114  49.819  1.00  8.42          C
ANISOU15462  CD2 TYR D 113     1228   1140    829    109    301   -275      C
ATOM  15464  C   TYR D 113      81.712  35.466  46.863  1.00 10.45          C
ANISOU15464  C   TYR D 113     1270   1430   1268     54     21     33      C
ATOM  15465  O   TYR D 113      81.007  36.453  46.824  1.00  8.60          O
ANISOU15465  O   TYR D 113      928   1216   1120    247   -232     30      O
ATOM  15466  N   GLY D 114      81.321  34.277  46.451  1.00  9.07          N
ANISOU15466  N   GLY D 114     1061   1236   1146     85     96    -59      N
ATOM  15468  CA  GLY D 114      79.930  34.028  46.232  1.00  9.92          C
ANISOU15468  CA  GLY D 114     1300   1265   1201    -21    -46     17      C
ATOM  15471  C   GLY D 114      79.602  32.782  45.492  1.00  9.45          C
ANISOU15471  C   GLY D 114     1221   1187   1180     31    -29    -10      C
ATOM  15472  O   GLY D 114      80.498  32.064  45.067  1.00  8.37          O
ANISOU15472  O   GLY D 114      845   1393    939    -72    -32   -203      O
ATOM  15473  N   HIS D 115      78.294  32.576  45.333  1.00  8.61          N
ANISOU15473  N   HIS D 115     1040   1134   1097     96    -46     44      N
ATOM  15475  CA  HIS D 115      77.731  31.385  44.699  1.00  8.42          C
ANISOU15475  CA  HIS D 115      967   1155   1074     59    -58    -16      C
ATOM  15477  CB  HIS D 115      76.191  31.289  44.865  1.00  9.01          C
ANISOU15477  CB  HIS D 115     1136   1291    996    -16     63    -37      C
ATOM  15480  CG  HIS D 115      75.597  30.123  44.126  1.00  7.23          C
ANISOU15480  CG  HIS D 115      699    907   1141     16    156     49      C
ATOM  15481  ND1 HIS D 115      75.952  28.807  44.399  1.00  6.20          N
ANISOU15481  ND1 HIS D 115     1019    622    713    111    182    -40      N
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ATOM  15483  CE1 HIS D 115      75.263  28.004  43.615  1.00  7.81           C
ANISOU15483  CE1 HIS D 115       948    855    1162    126     20    -18      C
ATOM  15485  NE2 HIS D 115      74.427  28.727  42.890  1.00  5.41           N
ANISOU15485  NE2 HIS D 115       712    561     781    304    307     18      N
ATOM  15487  CD2 HIS D 115      74.679  30.062  43.137  1.00  8.28           C
ANISOU15487  CD2 HIS D 115      1326    718    1101    116   -100     29      C
ATOM  15489  C   HIS D 115      78.109  31.325  43.235  1.00  8.57           C
ANISOU15489  C   HIS D 115      1036   1184    1035     17    -95    -21      C
ATOM  15490  O   HIS D 115      77.961  32.316  42.490  1.00  9.04           O
ANISOU15490  O   HIS D 115      1181   1121    1129    -65      7   -186      O
ATOM  15491  N   ASP D 116      78.714  30.190  42.872  1.00  9.73           N
ANISOU15491  N   ASP D 116      1280   1334    1080   -113    -62     44      N
ATOM  15493  CA  ASP D 116      79.116  29.893  41.522  1.00 10.85           C
ANISOU15493  CA  ASP D 116      1380   1380    1361     -5    -33    -53      C
ATOM  15495  CB  ASP D 116      77.854  29.934  40.640  1.00 10.53           C
ANISOU15495  CB  ASP D 116      1238   1454    1308     58   -116    -49      C
ATOM  15498  CG  ASP D 116      77.076  28.609  40.625  1.00 14.06           C
ANISOU15498  CG  ASP D 116      1784   1810    1749    -64    -63     95      C
ATOM  15499  OD1 ASP D 116      77.291  27.702  41.478  1.00 13.77           O
ANISOU15499  OD1 ASP D 116      1653   1897    1682    189     31    -89      O
ATOM  15500  OD2 ASP D 116      76.166  28.378  39.780  1.00 15.52           O
ANISOU15500  OD2 ASP D 116      1849   2164    1883   -166   -257    423      O
ATOM  15501  C   ASP D 116      80.253  30.828  41.005  1.00 10.86           C
ANISOU15501  C   ASP D 116      1370   1369    1386     47     12     36      C
ATOM  15502  O   ASP D 116      80.401  31.056  39.797  1.00 10.52           O
ANISOU15502  O   ASP D 116      1353   1345    1300    165    -67     97      O
ATOM  15503  N   PHE D 117      81.055  31.356  41.931  1.00 11.53           N
ANISOU15503  N   PHE D 117      1380   1472    1525     71     -2     50      N
ATOM  15505  CA  PHE D 117      82.303  32.073  41.560  1.00 12.16           C
ANISOU15505  CA  PHE D 117      1535   1509    1574    -32    -10     44      C
ATOM  15507  CB  PHE D 117      83.034  32.528  42.824  1.00 12.57           C
ANISOU15507  CB  PHE D 117      1586   1577    1613     48    -10    -31      C
ATOM  15510  CG  PHE D 117      84.206  33.470  42.591  1.00 11.44           C
ANISOU15510  CG  PHE D 117      1417   1541    1387     44    -34   -110      C
ATOM  15511  CD1 PHE D 117      84.115  34.557  41.742  1.00 13.84           C
ANISOU15511  CD1 PHE D 117      1687   1715    1854     -2   -149   -103      C
ATOM  15513  CE1 PHE D 117      85.155  35.432  41.529  1.00 14.37           C
ANISOU15513  CE1 PHE D 117      1689   1756    2012    101     87    120      C
ATOM  15515  CZ  PHE D 117      86.353  35.237  42.175  1.00 14.26           C
ANISOU15515  CZ  PHE D 117      1740   1941    1736   -119    -37     85      C
ATOM  15517  CE2 PHE D 117      86.466  34.170  43.098  1.00 14.03           C
ANISOU15517  CE2 PHE D 117      1665   1595    2068     29     70    -65      C
ATOM  15519  CD2 PHE D 117      85.379  33.286  43.293  1.00 11.27           C
ANISOU15519  CD2 PHE D 117      1312   1601    1368    117     81    -63      C
ATOM  15521  C   PHE D 117      83.218  31.153  40.731  1.00 12.53           C
ANISOU15521  C   PHE D 117      1515   1605    1641     -8    -91     34      C
ATOM  15522  O   PHE D 117      83.913  31.619  39.778  1.00 13.20           O
ANISOU15522  O   PHE D 117      1826   1522    1664    120      2    115      O
ATOM  15523  N   HIS D 118      83.247  29.852  41.060  1.00 13.03           N
ANISOU15523  N   HIS D 118      1625   1671    1651    -13    -97     57      N
ATOM  15525  CA  HIS D 118      84.098  28.947  40.308  1.00 14.31           C
ANISOU15525  CA  HIS D 118      1829   1814    1793     22    -47     56      C
ATOM  15527  CB  HIS D 118      84.237  27.562  40.982  1.00 16.00           C
ANISOU15527  CB  HIS D 118      2063   2038    1977    -34    111     100      C
ATOM  15530  CG  HIS D 118      83.217  26.570  40.606  1.00 20.20           C
ANISOU15530  CG  HIS D 118      2584   2583    2507    -64   -209     35      C
ATOM  15531  ND1 HIS D 118      82.350  26.076  41.566  1.00 24.31           N
ANISOU15531  ND1 HIS D 118      2958   3220    3056     29    158    -62      N
ATOM  15533  CE1 HIS D 118      81.667  25.066  41.058  1.00 23.57           C
ANISOU15533  CE1 HIS D 118      2980   2872    3104     36    -83    -16      C
ATOM  15535  NE2 HIS D 118      82.141  24.823  39.845  1.00 25.04           N
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ANISOU15535	NE2	HIS	D	118	3038	3145	3331	-64	74	-28		N
ATOM 15537	CD2	HIS	D	118	83.242	25.627	39.633	1.00	23.54			C
ANISOU15537	CD2	HIS	D	118	3066	2815	3061	93	56	-150		C
ATOM 15539	C	HIS	D	118	83.711	28.869	38.832	1.00	13.65			C
ANISOU15539	C	HIS	D	118	1723	1704	1758	-49	32	-9		C
ATOM 15540	O	HIS	D	118	84.580	28.796	37.966	1.00	14.09			O
ANISOU15540	O	HIS	D	118	1815	1752	1784	-208	122	48		O
ATOM 15541	N	GLU	D	119	82.420	28.913	38.546	1.00	13.44			N
ANISOU15541	N	GLU	D	119	1740	1611	1754	-11	4	53		N
ATOM 15543	CA	GLU	D	119	81.967	28.860	37.190	1.00	13.71			C
ANISOU15543	CA	GLU	D	119	1716	1787	1704	-28	32	42		C
ATOM 15545	CB	GLU	D	119	80.436	28.531	37.079	1.00	14.49			C
ANISOU15545	CB	GLU	D	119	1784	1889	1832	-78	32	8		C
ATOM 15548	CG	GLU	D	119	80.031	27.092	37.448	1.00	14.57			C
ANISOU15548	CG	GLU	D	119	1980	1825	1730	-38	96	-38		C
ATOM 15551	CD	GLU	D	119	79.727	26.813	38.925	1.00	15.51			C
ANISOU15551	CD	GLU	D	119	2224	1888	1780	-131	-50	-27		C
ATOM 15552	OE1	GLU	D	119	80.083	27.614	39.789	1.00	12.17			O
ANISOU15552	OE1	GLU	D	119	2148	897	1577	-147	-68	188		O
ATOM 15553	OE2	GLU	D	119	79.147	25.709	39.215	1.00	16.54			O
ANISOU15553	OE2	GLU	D	119	2091	2122	2071	-91	199	53		O
ATOM 15554	C	GLU	D	119	82.230	30.194	36.498	1.00	13.46			C
ANISOU15554	C	GLU	D	119	1656	1713	1744	-105	60	41		C
ATOM 15555	O	GLU	D	119	82.547	30.213	35.305	1.00	11.96			O
ANISOU15555	O	GLU	D	119	1358	1594	1589	-150	179	251		O
ATOM 15556	N	LEU	D	120	82.025	31.293	37.203	1.00	14.15			N
ANISOU15556	N	LEU	D	120	1739	1829	1806	-145	110	143		N
ATOM 15558	CA	LEU	D	120	82.307	32.621	36.624	1.00	14.37			C
ANISOU15558	CA	LEU	D	120	1837	1825	1796	-29	-53	138		C
ATOM 15560	CB	LEU	D	120	82.044	33.677	37.687	1.00	15.13			C
ANISOU15560	CB	LEU	D	120	1866	1956	1927	52	-25	128		C
ATOM 15563	CG	LEU	D	120	82.489	35.101	37.419	1.00	17.51			C
ANISOU15563	CG	LEU	D	120	2353	2133	2165	-23	65	73		C
ATOM 15565	CD1	LEU	D	120	81.801	35.366	36.137	1.00	21.59			C
ANISOU15565	CD1	LEU	D	120	2897	2609	2697	-66	-126	152		C
ATOM 15569	CD2	LEU	D	120	82.082	36.143	38.461	1.00	17.90			C
ANISOU15569	CD2	LEU	D	120	2448	1995	2356	20	-209	115		C
ATOM 15573	C	LEU	D	120	83.796	32.670	36.191	1.00	14.11			C
ANISOU15573	C	LEU	D	120	1763	1858	1738	23	89	125		C
ATOM 15574	O	LEU	D	120	84.175	33.222	35.106	1.00	13.11			O
ANISOU15574	O	LEU	D	120	1653	1714	1614	-65	1	185		O
ATOM 15575	N	LEU	D	121	84.671	32.114	37.036	1.00	13.04			N
ANISOU15575	N	LEU	D	121	1603	1731	1621	-20	83	114		N
ATOM 15577	CA	LEU	D	121	86.121	32.130	36.700	1.00	13.96			C
ANISOU15577	CA	LEU	D	121	1727	1827	1747	26	96	31		C
ATOM 15579	CB	LEU	D	121	86.982	31.692	37.870	1.00	13.46			C
ANISOU15579	CB	LEU	D	121	1595	1853	1663	36	70	5		C
ATOM 15582	CG	LEU	D	121	86.897	32.647	39.089	1.00	13.40			C
ANISOU15582	CG	LEU	D	121	1523	1647	1918	9	-140	6		C
ATOM 15584	CD1	LEU	D	121	87.216	31.984	40.395	1.00	14.50			C
ANISOU15584	CD1	LEU	D	121	1815	1771	1922	-212	69	46		C
ATOM 15588	CD2	LEU	D	121	87.777	33.872	38.859	1.00	13.43			C
ANISOU15588	CD2	LEU	D	121	1676	1664	1760	-73	-32	43		C
ATOM 15592	C	LEU	D	121	86.397	31.208	35.516	1.00	15.37			C
ANISOU15592	C	LEU	D	121	1957	1982	1898	-13	101	16		C
ATOM 15593	O	LEU	D	121	87.192	31.553	34.623	1.00	13.73			O
ANISOU15593	O	LEU	D	121	1786	1707	1723	81	353	-125		O
ATOM 15594	N	GLY	D	122	85.777	30.020	35.543	1.00	16.28			N
ANISOU15594	N	GLY	D	122	2189	1944	2052	-8	114	-17		N
ATOM 15596	CA	GLY	D	122	85.896	29.069	34.458	1.00	18.89			C
ANISOU15596	CA	GLY	D	122	2468	2354	2355	-40	17	-28		C

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ATOM  15599  C   GLY D 122      85.479  29.662  33.143  1.00 19.26           C
ANISOU15599  C   GLY D 122    2522   2383   2410    -68     28    -17       C
ATOM  15600  O   GLY D 122      86.164  29.507  32.139  1.00 20.50           O
ANISOU15600  O   GLY D 122    2663   2572   2550   -129    119   -192       O
ATOM  15601  N   SER D 123      84.356  30.340  33.126  1.00 18.95           N
ANISOU15601  N   SER D 123    2358   2407   2436   -125     90    -44       N
ATOM  15603  CA  SER D 123      83.947  30.974  31.900  1.00 20.93           C
ANISOU15603  CA  SER D 123    2625   2647   2679    -79     -4    -37       C
ATOM  15605  CB  SER D 123      82.592  31.598  32.093  1.00 21.46           C
ANISOU15605  CB  SER D 123    2641   2731   2780    -79     38     18       C
ATOM  15608  OG  SER D 123      81.743  30.528  32.486  1.00 23.87           O
ANISOU15608  OG  SER D 123    2974   2901   3192   -235     93     82       O
ATOM  15610  C   SER D 123      84.965  31.989  31.377  1.00 20.92           C
ANISOU15610  C   SER D 123    2605   2754   2586    -97     22    -21       C
ATOM  15611  O   SER D 123      85.218  32.042  30.167  1.00 21.68           O
ANISOU15611  O   SER D 123    2734   3005   2495   -107   -187   -195       O
ATOM  15612  N   ALA D 124      85.562  32.799  32.258  1.00 19.51           N
ANISOU15612  N   ALA D 124    2532   2502   2377    -81     41    -73       N
ATOM  15614  CA  ALA D 124      86.543  33.747  31.760  1.00 19.42           C
ANISOU15614  CA  ALA D 124    2537   2471   2370    -51    -34    -20       C
ATOM  15616  CB  ALA D 124      86.844  34.884  32.793  1.00 19.42           C
ANISOU15616  CB  ALA D 124    2594   2416   2365    -15     54    -24       C
ATOM  15620  C   ALA D 124      87.819  33.050  31.369  1.00 19.74           C
ANISOU15620  C   ALA D 124    2617   2467   2416    -63     35    -79       C
ATOM  15622  N   SER D 125      88.225  32.025  32.095  1.00 21.12           N
ANISOU15622  N   SER D 125    2781   2704   2540    -36      9    -55       N
ATOM  15624  CA  SER D 125      89.490  31.390  31.774  1.00 23.17           C
ANISOU15624  CA  SER D 125    2945   2936   2923    -33     21    -25       C
ATOM  15626  CB  SER D 125      89.961  30.500  32.920  1.00 24.07           C
ANISOU15626  CB  SER D 125    3117   3040   2987    -59    -38     24       C
ATOM  15629  OG  SER D 125      89.514  29.173  32.774  1.00 26.65           O
ANISOU15629  OG  SER D 125    3387   3443   3296    -24   -194    -92       O
ATOM  15633  N   GLN D 126      88.277  30.268  30.005  1.00 26.06           N
ANISOU15633  N   GLN D 126    3314   3329   3256    -78     61    -26       N
ATOM  15640  CG  GLN D 126      87.309  27.336  29.576  1.00 32.72           C
ANISOU15640  CG  GLN D 126    4227   4092   4111     37    -13      2       C
ATOM  15643  CD  GLN D 126      86.129  26.544  30.046  1.00 37.36           C
ANISOU15643  CD  GLN D 126    4703   4739   4754   -148     34     45       C
ATOM  15644  OE1 GLN D 126      84.983  26.961  29.862  1.00 40.15           O
ANISOU15644  OE1 GLN D 126    4981   5167   5106     46     21     11       O
ATOM  15645  NE2 GLN D 126      86.397  25.401  30.672  1.00 40.01           N
ANISOU15645  NE2 GLN D 126    5177   4898   5128      1    -84     51       N
ATOM  15751  CA  PHE D 134      84.632  42.192  35.832  1.00 10.46           C
ANISOU15751  CA  PHE D 134    1302   1432   1238    -74    -62    -15       C
ATOM  15753  CB  PHE D 134      84.703  41.176  36.950  1.00 12.21           C
ANISOU15753  CB  PHE D 134    1581   1540   1517    -90    -59     -5       C
ATOM  15756  CG  PHE D 134      85.106  39.837  36.463  1.00 15.32           C
ANISOU15756  CG  PHE D 134    2059   1864   1896     33    144    -71       C
ATOM  15757  CD1 PHE D 134      86.455  39.513  36.347  1.00 18.75           C
ANISOU15757  CD1 PHE D 134    2272   2262   2590     33   -190   -101       C
ATOM  15759  CE1 PHE D 134      86.860  38.325  35.794  1.00 19.22           C
ANISOU15759  CE1 PHE D 134    2492   2280   2528    146    -66     79       C
ATOM  15761  CZ  PHE D 134      85.917  37.427  35.365  1.00 19.54           C
ANISOU15761  CZ  PHE D 134    2609   2161   2653     95   -224     54       C
ATOM  15763  CE2 PHE D 134      84.563  37.730  35.447  1.00 20.85           C
ANISOU15763  CE2 PHE D 134    2773   2374   2774     53    102    -29       C
ATOM  15765  CD2 PHE D 134      84.152  38.976  35.970  1.00 17.98           C
ANISOU15765  CD2 PHE D 134    2496   2122   2213   -103     -4    -28       C
ATOM  15783  CB  TYR D 136      81.679  44.948  41.151  1.00  8.24           C
ANISOU15783  CB  TYR D 136     972   1011   1145   -148      4     96       C
ATOM  15786  CG  TYR D 136      81.061  44.511  42.473  1.00  8.30           C
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ANISOU15786	CG	TYR	D	136	1131	1014	1010	213	-280	234		C
ATOM 15787	CD1	TYR	D	136	80.516	43.218	42.622	1.00	9.08			C
ANISOU15787	CD1	TYR	D	136	1072	1289	1087	2	-199	0		C
ATOM 15789	CE1	TYR	D	136	80.073	42.765	43.807	1.00	9.63			C
ANISOU15789	CE1	TYR	D	136	1350	832	1476	-34	117	30		C
ATOM 15791	CZ	TYR	D	136	80.246	43.509	44.958	1.00	8.94			C
ANISOU15791	CZ	TYR	D	136	855	1312	1229	-1	-189	-40		C
ATOM 15792	OH	TYR	D	136	79.775	43.024	46.166	1.00	10.79			O
ANISOU15792	OH	TYR	D	136	1283	1624	1192	-290	-118	-60		O
ATOM 15794	CE2	TYR	D	136	80.743	44.789	44.861	1.00	7.43			C
ANISOU15794	CE2	TYR	D	136	445	1162	1213	-17	-112	176		C
ATOM 15796	CD2	TYR	D	136	81.189	45.268	43.585	1.00	10.13			C
ANISOU15796	CD2	TYR	D	136	1160	1424	1263	235	-192	42		C
ATOM 16347	CA	THR	D	172	87.664	44.843	40.016	1.00	9.27			C
ANISOU16347	CA	THR	D	172	1033	1306	1182	23	41	53		C
ATOM 16349	CB	THR	D	172	86.843	43.644	40.524	1.00	9.86			C
ANISOU16349	CB	THR	D	172	1056	1379	1309	12	-64	55		C
ATOM 16351	OG1	THR	D	172	87.059	42.487	39.688	1.00	11.86			O
ANISOU16351	OG1	THR	D	172	1330	1721	1453	-46	-276	-11		O
ATOM 16353	CG2	THR	D	172	85.341	43.951	40.514	1.00	11.33			C
ANISOU16353	CG2	THR	D	172	1429	1446	1430	61	33	126		C
ATOM 16359	N	GLY	D	173	89.820	43.979	40.764	1.00	10.37			N
ANISOU16359	N	GLY	D	173	1208	1466	1263	20	98	90		N
ATOM 16364	C	GLY	D	173	91.468	42.150	40.212	1.00	11.90			C
ANISOU16364	C	GLY	D	173	1514	1540	1465	20	-43	62		C
ATOM 16365	O	GLY	D	173	92.252	41.407	40.840	1.00	11.81			O
ANISOU16365	O	GLY	D	173	1118	1789	1580	161	-105	47		O
ATOM 16366	N	LEU	D	174	90.825	41.753	39.114	1.00	11.48			N
ANISOU16366	N	LEU	D	174	1474	1519	1367	11	-91	62		N
ATOM 16368	CA	LEU	D	174	90.932	40.406	38.574	1.00	11.20			C
ANISOU16368	CA	LEU	D	174	1451	1499	1303	20	-53	84		C
ATOM 16370	CB	LEU	D	174	89.774	39.510	39.097	1.00	11.10			C
ANISOU16370	CB	LEU	D	174	1256	1622	1339	-1	-100	65		C
ATOM 16373	CG	LEU	D	174	89.745	38.053	38.599	1.00	13.12			C
ANISOU16373	CG	LEU	D	174	1510	1753	1719	44	-82	19		C
ATOM 16375	CD1	LEU	D	174	91.043	37.248	38.882	1.00	12.18			C
ANISOU16375	CD1	LEU	D	174	1541	1289	1798	-34	-155	183		C
ATOM 16379	CD2	LEU	D	174	88.542	37.297	39.098	1.00	16.16			C
ANISOU16379	CD2	LEU	D	174	2140	2104	1895	-105	6	98		C
ATOM 16383	C	LEU	D	174	90.827	40.541	37.063	1.00	11.00			C
ANISOU16383	C	LEU	D	174	1396	1438	1343	1	-25	29		C
ATOM 16384	O	LEU	D	174	89.816	40.980	36.543	1.00	11.81			O
ANISOU16384	O	LEU	D	174	1654	1572	1261	279	-121	120		O
ATOM 16414	CD1	PHE	D	176	89.923	36.340	34.282	1.00	14.36			C
ANISOU16414	CD1	PHE	D	176	1963	1550	1942	-4	159	43		C
ATOM 16416	CE1	PHE	D	176	89.597	35.620	35.407	1.00	15.28			C
ANISOU16416	CE1	PHE	D	176	2005	1945	1856	4	212	50		C
ATOM 16418	CZ	PHE	D	176	90.003	34.310	35.547	1.00	14.97			C
ANISOU16418	CZ	PHE	D	176	2044	1834	1806	31	36	22		C
ATOM 16420	CE2	PHE	D	176	90.774	33.736	34.575	1.00	14.53			C
ANISOU16420	CE2	PHE	D	176	1964	1669	1885	-40	56	45		C
ATOM 16422	CD2	PHE	D	176	91.085	34.447	33.430	1.00	14.76			C
ANISOU16422	CD2	PHE	D	176	1882	1807	1915	33	127	72		C
ATOM 17024	CB	GLU	D	214	81.723	39.400	32.952	1.00	14.76			C
ANISOU17024	CB	GLU	D	214	1869	1902	1836	-44	16	-18		C
ATOM 17052	C	ILE	D	215	79.104	41.058	36.376	1.00	10.12			C
ANISOU17052	C	ILE	D	215	1160	1349	1335	13	28	-32		C
ATOM 17053	O	ILE	D	215	78.620	39.950	36.186	1.00	9.90			O
ANISOU17053	O	ILE	D	215	1504	1284	973	36	-49	106		O
ATOM 17054	N	MET	D	216	79.746	41.388	37.476	1.00	10.21			N
ANISOU17054	N	MET	D	216	1240	1370	1268	-114	92	-14		N

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ATOM  17056  CA  MET D 216      79.795  40.580  38.655  1.00 10.97           C
ANISOU17056  CA  MET D 216     1346   1380   1439     -6     28    -32       C
ATOM  17058  CB  MET D 216      81.086  40.796  39.385  1.00 13.21           C
ANISOU17058  CB  MET D 216     1749   1672   1597    -31    -47     63       C
ATOM  17061  CG  MET D 216      81.160  40.075  40.718  1.00 12.50           C
ANISOU17061  CG  MET D 216     1638   1609   1499    -60    -44    183       C
ATOM  17064  SD  MET D 216      82.853  40.115  41.404  1.00 13.17           S
ANISOU17064  SD  MET D 216     1370   1819   1812     52    -52    -33       S
ATOM  17065  CE  MET D 216      83.686  39.307  40.308  1.00 17.09           C
ANISOU17065  CE  MET D 216     2091   2339   2064    141     74    133       C
ATOM  17069  C   MET D 216      78.586  41.086  39.502  1.00 10.53           C
ANISOU17069  C   MET D 216     1298   1433   1270    -10     84    -10       C
ATOM  17070  O   MET D 216      78.595  42.174  40.074  1.00  9.66           O
ANISOU17070  O   MET D 216     1067   1237   1365    122    355     68       O
ATOM  17071  N   GLY D 217      77.583  40.262  39.596  1.00 10.64           N
ANISOU17071  N   GLY D 217     1407   1293   1340      0     21    -52       N
ATOM  17073  CA  GLY D 217      76.286  40.650  40.186  1.00 10.02           C
ANISOU17073  CA  GLY D 217     1220   1356   1229    -33     72    -22       C
ATOM  17076  C   GLY D 217      76.370  41.005  41.664  1.00 10.26           C
ANISOU17076  C   GLY D 217     1235   1432   1229    -16     62    -24       C
ATOM  17077  O   GLY D 217      77.307  40.574  42.368  1.00 10.90           O
ANISOU17077  O   GLY D 217     1320   1524   1296     18    103     61       O
ATOM  17078  N   ARG D 218      75.343  41.714  42.152  1.00  9.62           N
ANISOU17078  N   ARG D 218     1213   1268   1174    -21    -38    -41       N
ATOM  17080  CA  ARG D 218      75.300  42.189  43.549  1.00  9.84           C
ANISOU17080  CA  ARG D 218     1181   1311   1246     13     64     14       C
ATOM  17082  CB  ARG D 218      74.132  43.117  43.724  1.00  9.14           C
ANISOU17082  CB  ARG D 218     1199   1125   1146     39   -100    -40       C
ATOM  17100  C   ARG D 218      75.224  41.035  44.556  1.00  9.42           C
ANISOU17100  C   ARG D 218     1056   1260   1263     92     55     13       C
ATOM  17101  O   ARG D 218      75.447  41.229  45.716  1.00  9.80           O
ANISOU17101  O   ARG D 218     1126   1287   1310    145    339     10       O
ATOM  17102  N   GLY D 219      74.945  39.834  44.101  1.00  9.41           N
ANISOU17102  N   GLY D 219     1153   1170   1251      3     39     29       N
ATOM  17104  CA  GLY D 219      74.975  38.662  44.992  1.00 10.78           C
ANISOU17104  CA  GLY D 219     1468   1355   1272     42    -14    -73       C
ATOM  17107  C   GLY D 219      76.372  38.214  45.383  1.00  9.62           C
ANISOU17107  C   GLY D 219     1353   1146   1156    -22    -20    -81       C
ATOM  17108  O   GLY D 219      76.538  37.469  46.358  1.00 12.23           O
ANISOU17108  O   GLY D 219     1585   1700   1362    208    -10     51       O
ATOM  17109  N   TYR D 220      77.387  38.650  44.638  1.00  8.50           N
ANISOU17109  N   TYR D 220     1233   1130    866     45     -5    -67       N
ATOM  17111  CA  TYR D 220      78.741  38.381  45.035  1.00  8.93           C
ANISOU17111  CA  TYR D 220     1326   1044   1021      2     15     71       C
ATOM  17113  CB  TYR D 220      79.672  38.417  43.883  1.00  9.30           C
ANISOU17113  CB  TYR D 220     1095   1127   1310    121    -63     62       C
ATOM  17116  CG  TYR D 220      79.559  37.289  42.919  1.00  9.55           C
ANISOU17116  CG  TYR D 220     1183   1259   1183   -134    -54    -50       C
ATOM  17117  CD1 TYR D 220      78.944  37.495  41.697  1.00 11.63           C
ANISOU17117  CD1 TYR D 220     1295   1705   1417    -33     55      3       C
ATOM  17119  CE1 TYR D 220      78.840  36.486  40.773  1.00 10.42           C
ANISOU17119  CE1 TYR D 220     1055   1605   1298   -212    238    -68       C
ATOM  17121  CZ  TYR D 220      79.343  35.236  41.043  1.00 13.68           C
ANISOU17121  CZ  TYR D 220     1589   1915   1694    -31    119      6       C
ATOM  17122  OH  TYR D 220      79.173  34.260  40.070  1.00 16.65           O
ANISOU17122  OH  TYR D 220     1989   2444   1892    219    163    -247       O
ATOM  17124  CE2 TYR D 220      79.969  34.959  42.259  1.00 12.72           C
ANISOU17124  CE2 TYR D 220     1457   1554   1819    124    -87    -19       C
ATOM  17126  CD2 TYR D 220      80.063  36.010  43.210  1.00 14.00           C
ANISOU17126  CD2 TYR D 220     1639   1879   1798    173   -258    -125       C
ATOM  17128  C   TYR D 220      79.219  39.460  45.974  1.00  9.29           C
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ANISOU17128  C   TYR D 220     1285   1200   1043    -60     -8     40       C
ATOM  17129  O   TYR D 220      78.739  40.599  45.932  1.00  8.95           O
ANISOU17129  O   TYR D 220     1486   1208    706    -47     25    147       O
ATOM  17130  N   ALA D 221      80.171  39.097  46.809  1.00 10.54           N
ANISOU17130  N   ALA D 221     1430   1350   1222     29    -12    115       N
ATOM  17132  CA  ALA D 221      80.915  40.100  47.591  1.00 11.67           C
ANISOU17132  CA  ALA D 221     1519   1485   1427     -1     33     58       C
ATOM  17134  CB  ALA D 221      81.208  39.639  49.036  1.00 13.33           C
ANISOU17134  CB  ALA D 221     1815   1689   1558     90     30     59       C
ATOM  17138  C   ALA D 221      82.248  40.316  46.928  1.00 11.26           C
ANISOU17138  C   ALA D 221     1445   1525   1306    -17     16     92       C
ATOM  17139  O   ALA D 221      82.997  39.363  46.707  1.00 10.50           O
ANISOU17139  O   ALA D 221     1450   1341   1196   -233    293    116       O
ATOM  17140  N   TRP D 222      82.573  41.572  46.761  1.00 10.18           N
ANISOU17140  N   TRP D 222     1286   1393   1188    -80     16     48       N
ATOM  17142  CA  TRP D 222      83.880  42.007  46.261  1.00 10.95           C
ANISOU17142  CA  TRP D 222     1199   1593   1368      1     11     56       C
ATOM  17144  CB  TRP D 222      83.875  42.542  44.843  1.00 11.21           C
ANISOU17144  CB  TRP D 222     1257   1591   1410    -39    -13     68       C
ATOM  17147  CG  TRP D 222      85.231  43.127  44.491  1.00 10.60           C
ANISOU17147  CG  TRP D 222     1238   1599   1189     -6     62     79       C
ATOM  17148  CD1 TRP D 222      86.424  42.471  44.575  1.00 13.24           C
ANISOU17148  CD1 TRP D 222     1526   1769   1735     30     40     17       C
ATOM  17150  NE1 TRP D 222      87.447  43.319  44.232  1.00 12.16           N
ANISOU17150  NE1 TRP D 222     1387   1898   1333    118    211      4       N
ATOM  17152  CE2 TRP D 222      86.944  44.552  43.936  1.00 12.39           C
ANISOU17152  CE2 TRP D 222     1608   1662   1436     13    200    101       C
ATOM  17153  CD2 TRP D 222      85.554  44.486  44.115  1.00 10.71           C
ANISOU17153  CD2 TRP D 222     1416   1567   1084     21    -79     12       C
ATOM  17154  CE3 TRP D 222      84.801  45.624  43.825  1.00 12.02           C
ANISOU17154  CE3 TRP D 222     1432   1652   1483    -23    222     37       C
ATOM  17160  CZ2 TRP D 222      87.598  45.723  43.521  1.00 13.11           C
ANISOU17160  CZ2 TRP D 222     1718   1601   1660    -57    112    -87       C
ATOM  17162  C   TRP D 222      84.333  43.101  47.219  1.00 11.40           C
ANISOU17162  C   TRP D 222     1389   1494   1446    -19    129     47       C
ATOM  17163  O   TRP D 222      83.747  44.182  47.270  1.00 11.18           O
ANISOU17163  O   TRP D 222     1153   1578   1514    -53     84     69       O
ATOM  17164  N   LEU D 223      85.317  42.761  48.039  1.00 10.67           N
ANISOU17164  N   LEU D 223      986   1485   1580    151    142    -28       N
ATOM  17166  CA  LEU D 223      85.830  43.596  49.104  1.00 13.05           C
ANISOU17166  CA  LEU D 223     1548   1692   1715     77     71      3       C
ATOM  17168  CB  LEU D 223      85.705  42.886  50.389  1.00 13.78           C
ANISOU17168  CB  LEU D 223     1628   1836   1770     36     87    -50       C
ATOM  17171  CG  LEU D 223      84.283  42.494  50.695  1.00 14.22           C
ANISOU17171  CG  LEU D 223     1729   1930   1742    -16     36    -38       C
ATOM  17173  CD1 LEU D 223      84.200  41.818  52.105  1.00 16.38           C
ANISOU17173  CD1 LEU D 223     2112   2206   1905     44    106      1       C
ATOM  17177  CD2 LEU D 223      83.374  43.699  50.564  1.00 14.71           C
ANISOU17177  CD2 LEU D 223     1834   2014   1738    -12    180    181       C
ATOM  17181  C   LEU D 223      87.289  43.948  48.867  1.00 14.62           C
ANISOU17181  C   LEU D 223     1719   1967   1868     24     36     59       C
ATOM  17182  O   LEU D 223      88.004  43.175  48.239  1.00 15.86           O
ANISOU17182  O   LEU D 223     1776   2100   2149     75    103    168       O
ATOM  17183  N   ASP D 224      87.682  45.129  49.312  1.00 17.34           N
ANISOU17183  N   ASP D 224     2155   2372   2061     -7      7    -20       N
ATOM  17185  CA  ASP D 224      89.039  45.680  49.123  1.00 19.46           C
ANISOU17185  CA  ASP D 224     2428   2613   2351     -7    -59    -90       C
ATOM  17203  CG2 THR D 225      90.714  42.756  52.661  1.00 19.72           C
ANISOU17203  CG2 THR D 225     2592   2607   2294     90    124     -5       C
ATOM  17323  O   GLU D 233      83.967  42.453  57.169  1.00 10.64           O
ANISOU17323  O   GLU D 233     1370   1402   1270      6    -41    125       O
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ATOM  17324  N   ALA D 234      85.971  43.140  56.424  1.00  9.92           N
ANISOU17324  N   ALA D 234    1185   1258   1324    -50    18     1       N
ATOM  17326  CA  ALA D 234      86.198  41.869  55.728  1.00  9.91           C
ANISOU17326  CA  ALA D 234    1161   1305   1297    -33   -18    35       C
ATOM  17328  CB  ALA D 234      87.337  41.987  54.747  1.00  9.20           C
ANISOU17328  CB  ALA D 234     994   1309   1189     83   -61    37       C
ATOM  17332  C   ALA D 234      86.387  40.721  56.727  1.00  9.56           C
ANISOU17332  C   ALA D 234    1182   1184   1264    -25    16   -20       C
ATOM  17333  O   ALA D 234      85.864  39.641  56.501  1.00  9.49           O
ANISOU17333  O   ALA D 234    1211   1138   1257   -159   134   -57       O
ATOM  17334  N   GLY D 235      87.099  40.963  57.837  1.00  9.32           N
ANISOU17334  N   GLY D 235    1217   1055   1267     39    40   -38       N
ATOM  17336  CA  GLY D 235      87.228  39.971  58.862  1.00  9.85           C
ANISOU17336  CA  GLY D 235    1234   1316   1190    -62    -8    14       C
ATOM  17339  C   GLY D 235      85.894  39.550  59.457  1.00  9.55           C
ANISOU17339  C   GLY D 235    1104   1274   1247      3   -20    66       C
ATOM  17340  O   GLY D 235      85.631  38.347  59.656  1.00  9.98           O
ANISOU17340  O   GLY D 235    1023   1375   1392   -252   200   106       O
ATOM  17356  C   GLN D 236      82.969  39.394  59.233  1.00  9.90           C
ANISOU17356  C   GLN D 236    1364   1174   1223     30    -2    -8       C
ATOM  17357  O   GLN D 236      82.249  38.525  59.581  1.00  9.00           O
ANISOU17357  O   GLN D 236    1476   1127    814    -56  -162   172       O
ATOM  17358  N   PHE D 237      83.110  39.750  57.961  1.00 10.41           N
ANISOU17358  N   PHE D 237    1459   1407   1088    -78   -51    36       N
ATOM  17360  CA  PHE D 237      82.326  39.101  56.888  1.00 11.16           C
ANISOU17360  CA  PHE D 237    1485   1377   1378    -97    -9     7       C
ATOM  17362  CB  PHE D 237      82.584  39.817  55.570  1.00 13.02           C
ANISOU17362  CB  PHE D 237    1822   1596   1527    -99   -12    20       C
ATOM  17365  CG  PHE D 237      81.695  39.367  54.431  1.00 13.04           C
ANISOU17365  CG  PHE D 237    1842   1672   1440   -104   -91   214       C
ATOM  17366  CD1 PHE D 237      80.375  39.840  54.326  1.00 17.86           C
ANISOU17366  CD1 PHE D 237    2230   2389   2165   -187  -160    31       C
ATOM  17368  CE1 PHE D 237      79.570  39.443  53.278  1.00 17.98           C
ANISOU17368  CE1 PHE D 237    2216   2415   2199    -82   -69    19       C
ATOM  17370  CZ  PHE D 237      80.020  38.522  52.415  1.00 17.15           C
ANISOU17370  CZ  PHE D 237    2274   2347   1894   -105   -96  -102       C
ATOM  17372  CE2 PHE D 237      81.270  38.067  52.466  1.00 18.28           C
ANISOU17372  CE2 PHE D 237    2500   2291   2154    -39  -299   177       C
ATOM  17374  CD2 PHE D 237      82.157  38.508  53.512  1.00 17.71           C
ANISOU17374  CD2 PHE D 237    2752   1883   2094   -193  -189    94       C
ATOM  17376  C   PHE D 237      82.683  37.610  56.852  1.00 11.00           C
ANISOU17376  C   PHE D 237    1429   1445   1303    -23   -18    27       C
ATOM  17377  O   PHE D 237      81.792  36.740  56.926  1.00 11.74           O
ANISOU17377  O   PHE D 237    1499   1388   1571    -62  -136    36       O
ATOM  17378  N   ILE D 238      83.978  37.322  56.768  1.00 10.34           N
ANISOU17378  N   ILE D 238    1224   1297   1407      7   -20     3       N
ATOM  17380  CA  ILE D 238      84.496  35.934  56.802  1.00  9.68           C
ANISOU17380  CA  ILE D 238    1177   1232   1269    -61   -74   -40       C
ATOM  17382  CB  ILE D 238      86.050  35.926  56.566  1.00  9.49           C
ANISOU17382  CB  ILE D 238    1260   1190   1156     19    33    10       C
ATOM  17384  CG1 ILE D 238      86.370  36.507  55.187  1.00  9.12           C
ANISOU17384  CG1 ILE D 238    1246   1063   1153     16     8  -127       C
ATOM  17387  CD1 ILE D 238      85.738  35.752  54.097  1.00 10.39           C
ANISOU17387  CD1 ILE D 238    1148   1487   1313   -394    11    44       C
ATOM  17391  CG2 ILE D 238      86.578  34.517  56.744  1.00 10.22           C
ANISOU17391  CG2 ILE D 238    1080   1424   1378    135    -1  -138       C
ATOM  17395  C   ILE D 238      84.124  35.193  58.062  1.00  9.64           C
ANISOU17395  C   ILE D 238    1158   1238   1264     17    44  -108       C
ATOM  17396  O   ILE D 238      83.667  34.023  58.023  1.00 10.60           O
ANISOU17396  O   ILE D 238    1635   1086   1306     -6   203  -209       O
ATOM  17397  N   ALA D 239      84.230  35.860  59.205  1.00  8.72           N
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ANISOU17397	N	ALA	D	239	1119	1073	1120	-90	-265	-66		N
ATOM 17399	CA	ALA	D	239	83.832	35.199	60.434	1.00	8.91			C
ANISOU17399	CA	ALA	D	239	972	1190	1222	26	6	-75		C
ATOM 17401	CB	ALA	D	239	84.145	36.075	61.650	1.00	9.70			C
ANISOU17401	CB	ALA	D	239	1055	1285	1346	-41	-117	-82		C
ATOM 17405	C	ALA	D	239	82.392	34.765	60.461	1.00	8.94			C
ANISOU17405	C	ALA	D	239	1137	1099	1161	-69	-7	-101		C
ATOM 17406	O	ALA	D	239	82.072	33.664	60.912	1.00	10.83			O
ANISOU17406	O	ALA	D	239	1489	1328	1297	-16	116	-148		O
ATOM 17407	N	THR	D	240	81.529	35.637	60.018	1.00	7.67			N
ANISOU17407	N	THR	D	240	908	984	1021	-119	-19	-7		N
ATOM 17409	CA	THR	D	240	80.127	35.326	60.030	1.00	9.37			C
ANISOU17409	CA	THR	D	240	1124	1086	1349	-13	-116	-113		C
ATOM 17411	CB	THR	D	240	79.340	36.571	59.619	1.00	9.96			C
ANISOU17411	CB	THR	D	240	1150	1162	1471	-8	28	-82		C
ATOM 17415	CG2	THR	D	240	77.837	36.220	59.476	1.00	9.38			C
ANISOU17415	CG2	THR	D	240	1144	932	1488	172	-102	-18		C
ATOM 17419	C	THR	D	240	79.840	34.084	59.138	1.00	8.95			C
ANISOU17419	C	THR	D	240	1091	1103	1203	-2	-153	-99		C
ATOM 17420	O	THR	D	240	79.115	33.191	59.546	1.00	9.27			O
ANISOU17420	O	THR	D	240	1167	1036	1319	-98	-359	-259		O
ATOM 17421	N	LEU	D	241	80.409	34.038	57.960	1.00	8.78			N
ANISOU17421	N	LEU	D	241	891	1102	1343	8	-170	-128		N
ATOM 17423	CA	LEU	D	241	80.168	32.879	57.093	1.00	10.06			C
ANISOU17423	CA	LEU	D	241	1243	1256	1324	46	-64	-95		C
ATOM 17425	CB	LEU	D	241	80.808	33.119	55.742	1.00	9.33			C
ANISOU17425	CB	LEU	D	241	1023	1197	1325	-116	9	-68		C
ATOM 17428	CG	LEU	D	241	80.149	34.154	54.845	1.00	13.37			C
ANISOU17428	CG	LEU	D	241	1648	1483	1946	-79	-28	-64		C
ATOM 17430	CD1	LEU	D	241	81.022	34.419	53.697	1.00	17.22			C
ANISOU17430	CD1	LEU	D	241	2408	2044	2088	24	1	40		C
ATOM 17434	CD2	LEU	D	241	78.751	33.692	54.349	1.00	15.10			C
ANISOU17434	CD2	LEU	D	241	1673	1912	2152	254	-336	11		C
ATOM 17438	C	LEU	D	241	80.742	31.608	57.697	1.00	8.96			C
ANISOU17438	C	LEU	D	241	1113	1115	1173	33	4	-107		C
ATOM 17439	O	LEU	D	241	80.102	30.557	57.718	1.00	8.90			O
ANISOU17439	O	LEU	D	241	963	1262	1156	-52	173	-69		O
ATOM 17440	N	GLU	D	242	81.995	31.679	58.147	1.00	9.68			N
ANISOU17440	N	GLU	D	242	1138	1142	1397	-101	1	-71		N
ATOM 17442	CA	GLU	D	242	82.670	30.480	58.686	1.00	9.14			C
ANISOU17442	CA	GLU	D	242	1147	1113	1210	-46	-33	-53		C
ATOM 17444	CB	GLU	D	242	84.155	30.731	58.948	1.00	9.67			C
ANISOU17444	CB	GLU	D	242	1203	1145	1324	-63	31	-74		C
ATOM 17447	CG	GLU	D	242	84.904	31.076	57.692	1.00	9.65			C
ANISOU17447	CG	GLU	D	242	1367	1208	1089	-97	-6	-44		C
ATOM 17450	CD	GLU	D	242	86.413	31.074	57.882	1.00	10.27			C
ANISOU17450	CD	GLU	D	242	1282	1385	1234	77	-32	69		C
ATOM 17451	OE1	GLU	D	242	86.862	31.189	59.054	1.00	11.33			O
ANISOU17451	OE1	GLU	D	242	1610	1426	1268	-24	-42	174		O
ATOM 17452	OE2	GLU	D	242	87.153	31.009	56.876	1.00	10.26			O
ANISOU17452	OE2	GLU	D	242	1603	1242	1053	50	-24	207		O
ATOM 17453	C	GLU	D	242	82.000	29.908	59.931	1.00	10.23			C
ANISOU17453	C	GLU	D	242	1289	1279	1319	-7	-9	-35		C
ATOM 17454	O	GLU	D	242	81.831	28.680	60.073	1.00	11.36			O
ANISOU17454	O	GLU	D	242	1594	1323	1396	-184	151	-96		O
ATOM 17455	N	ASN	D	243	81.602	30.796	60.826	1.00	10.17			N
ANISOU17455	N	ASN	D	243	1302	1250	1312	-103	0	-73		N
ATOM 17457	CA	ASN	D	243	80.889	30.381	62.011	1.00	10.80			C
ANISOU17457	CA	ASN	D	243	1447	1390	1266	-7	-4	15		C
ATOM 17459	CB	ASN	D	243	81.067	31.483	63.074	1.00	11.99			C
ANISOU17459	CB	ASN	D	243	1663	1426	1465	-69	105	25		C

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ATOM  17462  CG  ASN D 243      82.536  31.445  63.616  1.00 17.74           C
ANISOU17462  CG  ASN D 243    2228   2406   2105    -44   -205     31       C
ATOM  17464  ND2 ASN D 243      83.404  32.362  63.140  1.00 20.33           N
ANISOU17464  ND2 ASN D 243    2304   2776   2644   -142   -278     83       N
ATOM  17467  C   ASN D 243      79.478  29.829  61.792  1.00 10.18           C
ANISOU17467  C   ASN D 243    1366   1222   1279     48     21     71       C
ATOM  17468  O   ASN D 243      79.019  28.935  62.519  1.00 10.23           O
ANISOU17468  O   ASN D 243    1155   1331   1399    225     13    377       O
ATOM  17469  N   ARG D 244      78.789  30.286  60.760  1.00  9.26           N
ANISOU17469  N   ARG D 244    1248   1121   1149     17    -22     89       N
ATOM  17471  CA  ARG D 244      77.483  29.788  60.455  1.00  9.26           C
ANISOU17471  CA  ARG D 244    1298   1041   1176      0    -27     34       C
ATOM  17473  CB  ARG D 244      76.769  30.790  59.523  1.00 10.39           C
ANISOU17473  CB  ARG D 244    1359   1239   1349     37    -78      5       C
ATOM  17476  CG  ARG D 244      75.417  30.298  58.996  1.00 11.21           C
ANISOU17476  CG  ARG D 244    1637   1282   1339     47   -103     -6       C
ATOM  17479  CD  ARG D 244      74.430  30.138  60.075  1.00 11.36           C
ANISOU17479  CD  ARG D 244    1341   1381   1595    -33     51     39       C
ATOM  17482  NE  ARG D 244      73.085  30.023  59.624  1.00  9.24           N
ANISOU17482  NE  ARG D 244    1461   1237    810    284     49   -161       N
ATOM  17491  C   ARG D 244      77.586  28.425  59.761  1.00  8.39           C
ANISOU17491  C   ARG D 244    1119    991   1078     38    -63     16       C
ATOM  17492  O   ARG D 244      76.885  27.462  60.115  1.00  7.53           O
ANISOU17492  O   ARG D 244    1172    682   1004    -41     21    -26       O
ATOM  17493  N   GLN D 245      78.520  28.342  58.845  1.00  8.85           N
ANISOU17493  N   GLN D 245    1270    947   1144    -53    -41      2       N
ATOM  17495  CA  GLN D 245      78.627  27.167  57.941  1.00  9.62           C
ANISOU17495  CA  GLN D 245    1224   1151   1277    -46    -69    -52       C
ATOM  17497  CB  GLN D 245      79.170  27.564  56.609  1.00  9.49           C
ANISOU17497  CB  GLN D 245    1243   1131   1230    -66    -18    -79       C
ATOM  17500  CG  GLN D 245      78.366  28.541  55.821  1.00  9.07           C
ANISOU17500  CG  GLN D 245     841   1168   1435   -167     26      4       C
ATOM  17503  CD  GLN D 245      78.965  28.851  54.455  1.00  9.07           C
ANISOU17503  CD  GLN D 245    1264   1156   1023     88   -150     56       C
ATOM  17504  OE1 GLN D 245      80.090  28.387  54.106  1.00 11.03           O
ANISOU17504  OE1 GLN D 245    1585   1405   1201    114    -31    -45       O
ATOM  17505  NE2 GLN D 245      78.297  29.726  53.729  1.00  8.04           N
ANISOU17505  NE2 GLN D 245    1065   1189    801    362   -162     277       N
ATOM  17508  C   GLN D 245      79.464  25.976  58.437  1.00 10.04           C
ANISOU17508  C   GLN D 245    1220   1191   1401     25   -110     -43       C
ATOM  17509  O   GLN D 245      79.221  24.855  58.044  1.00  9.65           O
ANISOU17509  O   GLN D 245    1060   1283   1322     -8   -336     -52       O
ATOM  17510  N   GLY D 246      80.433  26.224  59.305  1.00  9.68           N
ANISOU17510  N   GLY D 246    1326   1155   1197      0   -215     -32       N
ATOM  17512  CA  GLY D 246      81.393  25.194  59.692  1.00 10.82           C
ANISOU17512  CA  GLY D 246    1328   1354   1427     62      6     -52       C
ATOM  17515  C   GLY D 246      82.319  24.851  58.542  1.00 10.90           C
ANISOU17515  C   GLY D 246    1296   1372   1471     33    -31     -61       C
ATOM  17516  O   GLY D 246      82.862  23.714  58.521  1.00 12.14           O
ANISOU17516  O   GLY D 246    1365   1437   1809    209    -24     100       O
ATOM  17517  N   LEU D 247      82.398  25.745  57.560  1.00  9.48           N
ANISOU17517  N   LEU D 247    1074   1099   1429     26    -75     -74       N
ATOM  17519  CA  LEU D 247      83.292  25.635  56.392  1.00 10.86           C
ANISOU17519  CA  LEU D 247    1336   1287   1502     17    -16     -55       C
ATOM  17521  CB  LEU D 247      82.524  25.527  55.076  1.00  9.90           C
ANISOU17521  CB  LEU D 247    1083   1241   1437    219     46      35       C
ATOM  17524  CG  LEU D 247      81.514  24.373  54.962  1.00 10.47           C
ANISOU17524  CG  LEU D 247    1364   1109   1505     86    -59      41       C
ATOM  17526  CD1 LEU D 247      80.631  24.451  53.736  1.00 10.65           C
ANISOU17526  CD1 LEU D 247    1417   1290   1336    -34     65    -165       C
ATOM  17530  CD2 LEU D 247      82.153  23.024  54.998  1.00 10.07           C
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ANISOU17530  CD2 LEU D 247     1268   1257   1299     89     23     42       C
ATOM  17534  C   LEU D 247      84.162  26.866  56.366  1.00 11.86           C
ANISOU17534  C   LEU D 247     1403   1410   1693     28     28    -63       C
ATOM  17535  O   LEU D 247      83.704  27.938  56.752  1.00 14.02           O
ANISOU17535  O   LEU D 247     1588   1546   2192   -194    104   -299       O
ATOM  17536  N   LYS D 248      85.383  26.756  55.875  1.00 10.39           N
ANISOU17536  N   LYS D 248     1145   1359   1441     44    -85    -85       N
ATOM  17538  CA  LYS D 248      86.263  27.878  55.871  1.00 12.66           C
ANISOU17538  CA  LYS D 248     1579   1509   1721     65    -19    -22       C
ATOM  17540  CB  LYS D 248      87.644  27.460  56.411  1.00 13.65           C
ANISOU17540  CB  LYS D 248     1494   1711   1980    -92   -155     -3       C
ATOM  17543  CG  LYS D 248      87.523  27.217  57.955  1.00 18.20           C
ANISOU17543  CG  LYS D 248     2272   2371   2270     25     26     82       C
ATOM  17546  CD  LYS D 248      88.857  27.304  58.829  1.00 23.61           C
ANISOU17546  CD  LYS D 248     2890   2952   3128    -46   -130     -7       C
ATOM  17549  CE  LYS D 248      88.575  27.730  60.314  1.00 25.17           C
ANISOU17549  CE  LYS D 248     3229   3182   3153   -114     28     59       C
ATOM  17552  NZ  LYS D 248      87.112  27.569  60.916  1.00 26.16           N
ANISOU17552  NZ  LYS D 248     3057   3409   3474   -121    -34    -90       N
ATOM  17556  C   LYS D 248      86.377  28.438  54.484  1.00 12.32           C
ANISOU17556  C   LYS D 248     1527   1557   1597     14    -26    -63       C
ATOM  17557  O   LYS D 248      86.264  27.696  53.563  1.00 13.54           O
ANISOU17557  O   LYS D 248     1686   1664   1794    -15     -6   -151       O
ATOM  17558  N   VAL D 249      86.521  29.759  54.356  1.00 12.28           N
ANISOU17558  N   VAL D 249     1533   1537   1595     13     21     27       N
ATOM  17560  CA  VAL D 249      86.761  30.428  53.063  1.00 10.47           C
ANISOU17560  CA  VAL D 249     1310   1340   1327     74    -30    -56       C
ATOM  17562  CB  VAL D 249      86.245  31.836  53.126  1.00 10.52           C
ANISOU17562  CB  VAL D 249     1205   1421   1369    -40    -15     12       C
ATOM  17564  CG1 VAL D 249      86.497  32.608  51.811  1.00  9.89           C
ANISOU17564  CG1 VAL D 249     1284   1252   1221    112   -177   -129       C
ATOM  17568  CG2 VAL D 249      84.696  31.786  53.566  1.00 12.00           C
ANISOU17568  CG2 VAL D 249     1357   1636   1567    211    -84   -167       C
ATOM  17572  C   VAL D 249      88.263  30.487  52.746  1.00  9.56           C
ANISOU17572  C   VAL D 249     1199   1149   1283      3    -57     40       C
ATOM  17573  O   VAL D 249      89.079  30.898  53.593  1.00 11.33           O
ANISOU17573  O   VAL D 249     1655   1212   1437    237     14     67       O
ATOM  17574  N   ALA D 250      88.623  30.110  51.521  1.00  8.67           N
ANISOU17574  N   ALA D 250     930   1076   1286     66    -51    -10       N
ATOM  17576  CA  ALA D 250      89.982  30.297  50.984  1.00  9.78           C
ANISOU17576  CA  ALA D 250     1258   1222   1233    -55    -33      5       C
ATOM  17578  CB  ALA D 250      90.320  31.801  50.906  1.00 10.37           C
ANISOU17578  CB  ALA D 250     1321   1308   1310    -74    -55    -53       C
ATOM  17582  C   ALA D 250      91.034  29.523  51.719  1.00 10.82           C
ANISOU17582  C   ALA D 250     1253   1360   1497    -27    -12    -16       C
ATOM  17583  O   ALA D 250      92.144  30.025  51.970  1.00 11.65           O
ANISOU17583  O   ALA D 250     1494   1365   1565    -62   -214   -214       O
ATOM  17584  N   CYS D 251      90.677  28.282  52.068  1.00 10.30           N
ANISOU17584  N   CYS D 251     1154   1303   1455    -49    -42     18       N
ATOM  17586  CA  CYS D 251      91.629  27.335  52.576  1.00 12.13           C
ANISOU17586  CA  CYS D 251     1544   1517   1548     14     66    -30       C
ATOM  17588  CB  CYS D 251      90.869  26.351  53.463  1.00 13.20           C
ANISOU17588  CB  CYS D 251     1639   1499   1876   -121   -126      4       C
ATOM  17591  SG  CYS D 251      91.783  24.962  54.066  1.00 16.67           S
ANISOU17591  SG  CYS D 251     2349   1960   2024    345    192   -257       S
ATOM  17592  C   CYS D 251      92.276  26.697  51.334  1.00 11.58           C
ANISOU17592  C   CYS D 251     1378   1478   1541     73    -31      5       C
ATOM  17593  O   CYS D 251      91.712  25.835  50.692  1.00 10.00           O
ANISOU17593  O   CYS D 251     949   1384   1466    230   -178    -85       O
ATOM  17594  N   PRO D 252      93.517  27.041  51.040  1.00 12.29           N
ANISOU17594  N   PRO D 252     1595   1509   1564     -1      6     41       N
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ATOM  17595  CA  PRO D 252      94.151  26.454  49.872  1.00 12.63           C
ANISOU17595  CA  PRO D 252    1599   1547   1652     24     23    -27       C
ATOM  17597  CB  PRO D 252      95.561  27.090  49.877  1.00 13.83           C
ANISOU17597  CB  PRO D 252    1695   1806   1752     43    -13    -68       C
ATOM  17600  CG  PRO D 252      95.455  28.314  50.664  1.00 13.60           C
ANISOU17600  CG  PRO D 252    1818   1682   1667    -32    -55     42       C
ATOM  17603  CD  PRO D 252      94.416  27.987  51.712  1.00 12.32           C
ANISOU17603  CD  PRO D 252    1449   1608   1622    118     33    -18       C
ATOM  17606  C   PRO D 252      94.262  24.907  49.917  1.00 12.73           C
ANISOU17606  C   PRO D 252    1661   1573   1602    -32     -2    -21       C
ATOM  17607  O   PRO D 252      94.139  24.252  48.855  1.00 10.69           O
ANISOU17607  O   PRO D 252    1340   1295   1425     81     30   -149       O
ATOM  17608  N   GLU D 253      94.479  24.359  51.112  1.00 11.57           N
ANISOU17608  N   GLU D 253    1372   1503   1521      6    -23    -12       N
ATOM  17610  CA  GLU D 253      94.599  22.950  51.231  1.00 11.36           C
ANISOU17610  CA  GLU D 253    1396   1443   1475     -9     26    -28       C
ATOM  17612  CB  GLU D 253      94.893  22.524  52.650  1.00 12.35           C
ANISOU17612  CB  GLU D 253    1568   1557   1564     43     25    -77       C
ATOM  17615  CG  GLU D 253      96.232  23.043  53.211  1.00 12.82           C
ANISOU17615  CG  GLU D 253    1513   1739   1619     69    -93     40       C
ATOM  17618  CD  GLU D 253      96.092  24.416  53.851  1.00 15.06           C
ANISOU17618  CD  GLU D 253    1960   1944   1818    -35     45     13       C
ATOM  17619  OE1 GLU D 253      95.088  25.122  53.577  1.00 15.96           O
ANISOU17619  OE1 GLU D 253    1869   2104   2091   -144    182    259       O
ATOM  17620  OE2 GLU D 253      96.962  24.794  54.663  1.00 18.42           O
ANISOU17620  OE2 GLU D 253    2356   2464   2178    -65   -199    199       O
ATOM  17621  C   GLU D 253      93.308  22.310  50.783  1.00 10.72           C
ANISOU17621  C   GLU D 253    1305   1401   1364      1     41    -31       C
ATOM  17622  O   GLU D 253      93.331  21.269  50.156  1.00  9.53           O
ANISOU17622  O   GLU D 253    1127   1246   1246    -16    189   -121       O
ATOM  17623  N   GLU D 254      92.171  22.882  51.169  1.00 10.16           N
ANISOU17623  N   GLU D 254    1339   1180   1339     30     26    -47       N
ATOM  17625  CA  GLU D 254      90.877  22.300  50.818  1.00 10.38           C
ANISOU17625  CA  GLU D 254    1240   1324   1377     28     61     13       C
ATOM  17627  CB  GLU D 254      89.723  23.078  51.490  1.00 10.49           C
ANISOU17627  CB  GLU D 254    1355   1240   1390     54     76     63       C
ATOM  17630  CG  GLU D 254      88.365  22.725  50.928  1.00  9.86           C
ANISOU17630  CG  GLU D 254    1286   1258   1202     32     19     74       C
ATOM  17633  CD  GLU D 254      87.178  23.264  51.732  1.00 10.27           C
ANISOU17633  CD  GLU D 254    1305   1124   1473    113    -35    109       C
ATOM  17634  OE1 GLU D 254      87.308  24.203  52.538  1.00 10.92           O
ANISOU17634  OE1 GLU D 254    1285   1650   1212    263     96    -62       O
ATOM  17635  OE2 GLU D 254      86.107  22.687  51.569  1.00 13.32           O
ANISOU17635  OE2 GLU D 254    1169   1985   1907    136   -129   -213       O
ATOM  17636  C   GLU D 254      90.663  22.354  49.347  1.00 10.66           C
ANISOU17636  C   GLU D 254    1252   1381   1417     65     92    -20       C
ATOM  17637  O   GLU D 254      90.253  21.385  48.703  1.00 10.32           O
ANISOU17637  O   GLU D 254     846   1578   1495    -44     38     83       O
ATOM  17638  N   ILE D 255      90.940  23.518  48.787  1.00 11.98           N
ANISOU17638  N   ILE D 255    1535   1477   1539     47     77      2       N
ATOM  17640  CA  ILE D 255      90.747  23.674  47.347  1.00 13.04           C
ANISOU17640  CA  ILE D 255    1712   1604   1635     22     43     -8       C
ATOM  17642  CB  ILE D 255      90.945  25.118  46.973  1.00 12.67           C
ANISOU17642  CB  ILE D 255    1597   1561   1655     25     71     14       C
ATOM  17644  CG1 ILE D 255      89.826  25.962  47.614  1.00 11.77           C
ANISOU17644  CG1 ILE D 255    1609   1434   1427     33     35    138       C
ATOM  17647  CD1 ILE D 255      90.109  27.449  47.533  1.00 14.33           C
ANISOU17647  CD1 ILE D 255    1918   1525   2000    -52    -21   -123       C
ATOM  17651  CG2 ILE D 255      90.892  25.312  45.454  1.00 14.11           C
ANISOU17651  CG2 ILE D 255    1799   1816   1744    -11     25    -54       C
ATOM  17655  C   ILE D 255      91.630  22.707  46.534  1.00 12.88           C
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ANISOU17655	C	ILE	D	255	1635	1627	1632	-4	42	21		C
ATOM 17656	O	ILE	D	255	91.155	22.120	45.522	1.00	13.53			O
ANISOU17656	O	ILE	D	255	1719	1564	1857	-46	139	-49		O
ATOM 17657	N	ALA	D	256	92.886	22.545	46.948	1.00	12.83			N
ANISOU17657	N	ALA	D	256	1707	1541	1627	-75	2	2		N
ATOM 17659	CA	ALA	D	256	93.806	21.660	46.270	1.00	12.69			C
ANISOU17659	CA	ALA	D	256	1620	1559	1643	-67	-16	28		C
ATOM 17661	CB	ALA	D	256	95.186	21.703	46.914	1.00	12.48			C
ANISOU17661	CB	ALA	D	256	1738	1365	1636	-20	-69	23		C
ATOM 17665	C	ALA	D	256	93.238	20.234	46.292	1.00	12.93			C
ANISOU17665	C	ALA	D	256	1687	1534	1689	-37	-17	-14		C
ATOM 17666	O	ALA	D	256	93.288	19.521	45.308	1.00	12.82			O
ANISOU17666	O	ALA	D	256	1507	1743	1619	-50	-120	-83		O
ATOM 17667	N	TYR	D	257	92.679	19.876	47.433	1.00	13.10			N
ANISOU17667	N	TYR	D	257	1667	1647	1664	-5	0	-29		N
ATOM 17669	CA	TYR	D	257	92.116	18.543	47.648	1.00	13.18			C
ANISOU17669	CA	TYR	D	257	1638	1692	1675	15	15	-1		C
ATOM 17671	CB	TYR	D	257	91.736	18.365	49.100	1.00	13.75			C
ANISOU17671	CB	TYR	D	257	1644	1828	1751	104	-75	7		C
ATOM 17674	CG	TYR	D	257	91.174	16.983	49.425	1.00	17.24			C
ANISOU17674	CG	TYR	D	257	2251	2168	2128	-113	-95	24		C
ATOM 17675	CD1	TYR	D	257	91.885	15.831	49.098	1.00	20.81			C
ANISOU17675	CD1	TYR	D	257	2661	2631	2613	-21	-8	-44		C
ATOM 17677	CE1	TYR	D	257	91.401	14.559	49.408	1.00	22.03			C
ANISOU17677	CE1	TYR	D	257	2942	2682	2745	-74	-75	0		C
ATOM 17679	CZ	TYR	D	257	90.184	14.416	50.069	1.00	23.82			C
ANISOU17679	CZ	TYR	D	257	3108	2974	2966	-67	-59	29		C
ATOM 17680	OH	TYR	D	257	89.700	13.137	50.359	1.00	26.01			O
ANISOU17680	OH	TYR	D	257	3521	3142	3219	-315	-26	114		O
ATOM 17682	CE2	TYR	D	257	89.454	15.514	50.412	1.00	23.15			C
ANISOU17682	CE2	TYR	D	257	2982	2924	2888	-96	65	-6		C
ATOM 17684	CD2	TYR	D	257	89.954	16.827	50.087	1.00	22.70			C
ANISOU17684	CD2	TYR	D	257	2871	2974	2778	-141	16	-29		C
ATOM 17686	C	TYR	D	257	90.908	18.337	46.751	1.00	13.24			C
ANISOU17686	C	TYR	D	257	1736	1722	1570	0	-20	33		C
ATOM 17687	O	TYR	D	257	90.816	17.345	46.018	1.00	13.63			O
ANISOU17687	O	TYR	D	257	1677	1955	1545	36	-133	59		O
ATOM 17688	N	ARG	D	258	89.993	19.279	46.798	1.00	14.41			N
ANISOU17688	N	ARG	D	258	1837	1979	1659	29	-31	-101		N
ATOM 17690	CA	ARG	D	258	88.755	19.216	46.003	1.00	16.24			C
ANISOU17690	CA	ARG	D	258	2019	2114	2037	26	-25	-17		C
ATOM 17692	CB	ARG	D	258	87.841	20.389	46.321	1.00	16.33			C
ANISOU17692	CB	ARG	D	258	2007	2111	2085	76	-8	-38		C
ATOM 17695	CG	ARG	D	258	87.223	20.284	47.697	1.00	16.95			C
ANISOU17695	CG	ARG	D	258	2270	2071	2099	-17	21	115		C
ATOM 17698	CD	ARG	D	258	86.167	21.326	48.019	1.00	19.07			C
ANISOU17698	CD	ARG	D	258	2335	2284	2626	-55	10	-44		C
ATOM 17701	NE	ARG	D	258	84.890	21.171	47.296	1.00	21.94			N
ANISOU17701	NE	ARG	D	258	2760	2903	2673	-38	-16	19		N
ATOM 17703	CZ	ARG	D	258	83.883	20.451	47.786	1.00	21.56			C
ANISOU17703	CZ	ARG	D	258	2746	2650	2796	-135	-103	-16		C
ATOM 17704	NH1	ARG	D	258	84.100	19.771	48.937	1.00	21.80			N
ANISOU17704	NH1	ARG	D	258	2764	2946	2573	-256	198	-103		N
ATOM 17707	NH2	ARG	D	258	82.718	20.327	47.128	1.00	19.77			N
ANISOU17707	NH2	ARG	D	258	2533	2291	2687	330	150	104		N
ATOM 17710	C	ARG	D	258	89.061	19.159	44.524	1.00	16.74			C
ANISOU17710	C	ARG	D	258	2120	2191	2048	64	-37	-34		C
ATOM 17711	O	ARG	D	258	88.360	18.475	43.790	1.00	17.91			O
ANISOU17711	O	ARG	D	258	2261	2300	2242	-83	-50	-101		O
ATOM 17712	N	GLN	D	259	90.106	19.853	44.091	1.00	17.73			N
ANISOU17712	N	GLN	D	259	2186	2297	2250	-8	-23	-16		N

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ATOM  17714  CA  GLN D 259      90.532  19.820  42.670  1.00 18.78           C
ANISOU17714  CA  GLN D 259    2419   2454   2261     35    -56    -14       C
ATOM  17716  CB  GLN D 259      91.365  21.036  42.348  1.00 19.38           C
ANISOU17716  CB  GLN D 259    2406   2694   2263    -28     -7    -11       C
ATOM  17719  CG  GLN D 259      90.705  22.309  42.640  1.00 24.77           C
ANISOU17719  CG  GLN D 259    3246   3077   3088     23    -49    -92       C
ATOM  17722  CD  GLN D 259      90.111  22.971  41.425  1.00 29.62           C
ANISOU17722  CD  GLN D 259    3908   3703   3641    114   -125     88       C
ATOM  17723  OE1 GLN D 259      89.694  22.307  40.451  1.00 32.16           O
ANISOU17723  OE1 GLN D 259    4119   4147   3953    -67   -212    -41       O
ATOM  17724  NE2 GLN D 259      90.059  24.276  41.472  1.00 31.75           N
ANISOU17724  NE2 GLN D 259    4181   3672   4209   -185    -93     38       N
ATOM  17727  C   GLN D 259      91.386  18.618  42.311  1.00 18.70           C
ANISOU17727  C   GLN D 259    2401   2462   2243     11    -37      0       C
ATOM  17728  O   GLN D 259      91.844  18.478  41.173  1.00 17.88           O
ANISOU17728  O   GLN D 259    2539   2212   2041     81   -131    -57       O
ATOM  17729  N   LYS D 260      91.669  17.788  43.309  1.00 18.20           N
ANISOU17729  N   LYS D 260    2365   2294   2257      9    -21      9       N
ATOM  17731  CA  LYS D 260      92.471  16.590  43.122  1.00 18.47           C
ANISOU17731  CA  LYS D 260    2282   2410   2324    -16      3     -7       C
ATOM  17733  CB  LYS D 260      91.831  15.692  42.021  1.00 18.97           C
ANISOU17733  CB  LYS D 260    2460   2415   2333     -9     59    -75       C
ATOM  17736  CG  LYS D 260      90.374  15.337  42.347  1.00 22.40           C
ANISOU17736  CG  LYS D 260    2735   2935   2840     -6    -17    -18       C
ATOM  17739  CD  LYS D 260      89.771  14.244  41.455  1.00 27.30           C
ANISOU17739  CD  LYS D 260    3441   3473   3458   -129    -39    -65       C
ATOM  17742  CE  LYS D 260      88.360  13.894  41.958  1.00 29.40           C
ANISOU17742  CE  LYS D 260    3618   3768   3784    -35     32      7       C
ATOM  17745  NZ  LYS D 260      87.761  15.051  42.698  1.00 31.87           N
ANISOU17745  NZ  LYS D 260    4090   3979   4040     14     77    -55       N
ATOM  17749  C   LYS D 260      93.950  16.893  42.841  1.00 17.06           C
ANISOU17749  C   LYS D 260    2143   2167   2172     27    -27      4       C
ATOM  17750  O   LYS D 260      94.610  16.067  42.293  1.00 16.73           O
ANISOU17750  O   LYS D 260    1990   2299   2066    -22      7    -68       O
ATOM  17751  N   TRP D 261      94.432  18.072  43.231  1.00 15.77           N
ANISOU17751  N   TRP D 261    1924   2098   1967     -7    -89     18       N
ATOM  17753  CA  TRP D 261      95.819  18.465  43.060  1.00 14.98           C
ANISOU17753  CA  TRP D 261    1883   1902   1905     -4    -15     28       C
ATOM  17755  CB  TRP D 261      95.976  19.981  43.081  1.00 12.87           C
ANISOU17755  CB  TRP D 261    1558   1643   1688    132     42    -29       C
ATOM  17758  CG  TRP D 261      95.340  20.621  41.879  1.00 15.22           C
ANISOU17758  CG  TRP D 261    1959   1919   1905      0    -41    -11       C
ATOM  17759  CD1 TRP D 261      94.902  20.003  40.728  1.00 15.27           C
ANISOU17759  CD1 TRP D 261    2001   1779   2020    -11   -133    -16       C
ATOM  17761  NE1 TRP D 261      94.359  20.932  39.865  1.00 15.73           N
ANISOU17761  NE1 TRP D 261    2005   1878   2093    -66   -193      2       N
ATOM  17763  CE2 TRP D 261      94.440  22.170  40.448  1.00 16.18           C
ANISOU17763  CE2 TRP D 261    2131   1924   2090      1    -65     35       C
ATOM  17764  CD2 TRP D 261      95.054  22.007  41.715  1.00 14.67           C
ANISOU17764  CD2 TRP D 261    1869   1776   1926    106    -60     34       C
ATOM  17765  CE3 TRP D 261      95.273  23.132  42.496  1.00 17.25           C
ANISOU17765  CE3 TRP D 261    2314   2113   2125     10     63    -32       C
ATOM  17767  CZ3 TRP D 261      94.836  24.384  42.005  1.00 17.69           C
ANISOU17767  CZ3 TRP D 261    2413   2221   2085    120    -78     52       C
ATOM  17769  CH2 TRP D 261      94.226  24.494  40.743  1.00 15.78           C
ANISOU17769  CH2 TRP D 261    2010   1992   1992     57    -16    -36       C
ATOM  17771  CZ2 TRP D 261      94.024  23.410  39.964  1.00 14.75           C
ANISOU17771  CZ2 TRP D 261    1679   1997   1928     43   -196     36       C
ATOM  17773  C   TRP D 261      96.682  17.840  44.141  1.00 15.05           C
ANISOU17773  C   TRP D 261    1877   1867   1974    -25    -38      0       C
ATOM  17774  O   TRP D 261      97.885  17.711  43.972  1.00 16.93           O
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ANISOU17774	O	TRP	D	261	2073	2116	2243	-42	-42	-21		O
ATOM 17775	N	ILE	D	262	96.073	17.486	45.252	1.00	14.77			N
ANISOU17775	N	ILE	D	262	1826	1927	1856	55	-18	-71		N
ATOM 17777	CA	ILE	D	262	96.718	16.669	46.275	1.00	15.00			C
ANISOU17777	CA	ILE	D	262	1896	1911	1891	45	2	-50		C
ATOM 17779	CB	ILE	D	262	97.106	17.493	47.502	1.00	14.27			C
ANISOU17779	CB	ILE	D	262	1830	1758	1832	31	45	9		C
ATOM 17781	CG1	ILE	D	262	95.857	18.144	48.129	1.00	13.25			C
ANISOU17781	CG1	ILE	D	262	1696	1646	1689	-6	-18	5		C
ATOM 17784	CD1	ILE	D	262	96.103	18.667	49.538	1.00	12.26			C
ANISOU17784	CD1	ILE	D	262	1379	1655	1625	139	50	44		C
ATOM 17788	CG2	ILE	D	262	98.189	18.517	47.139	1.00	13.17			C
ANISOU17788	CG2	ILE	D	262	1534	1859	1607	21	45	-6		C
ATOM 17792	C	ILE	D	262	95.739	15.557	46.653	1.00	16.33			C
ANISOU17792	C	ILE	D	262	2064	2078	2063	13	-2	-49		C
ATOM 17793	O	ILE	D	262	94.515	15.718	46.498	1.00	16.68			O
ANISOU17793	O	ILE	D	262	2072	2044	2220	44	50	-238		O
ATOM 17794	N	ASP	D	263	96.242	14.416	47.117	1.00	17.84			N
ANISOU17794	N	ASP	D	263	2232	2239	2307	77	48	-52		N
ATOM 17796	CA	ASP	D	263	95.338	13.365	47.591	1.00	18.82			C
ANISOU17796	CA	ASP	D	263	2426	2320	2403	-18	10	-6		C
ATOM 17804	C	ASP	D	263	95.084	13.412	49.102	1.00	18.82			C
ANISOU17804	C	ASP	D	263	2454	2306	2389	-25	13	34		C
ATOM 17805	O	ASP	D	263	95.560	14.281	49.813	1.00	17.56			O
ANISOU17805	O	ASP	D	263	2472	1963	2236	-51	121	101		O
ATOM 17806	N	ALA	D	264	94.351	12.426	49.593	1.00	19.63			N
ANISOU17806	N	ALA	D	264	2507	2425	2525	-110	30	4		N
ATOM 17808	CA	ALA	D	264	93.968	12.370	51.004	1.00	20.08			C
ANISOU17808	CA	ALA	D	264	2587	2521	2522	-68	10	25		C
ATOM 17843	N	LEU	D	267	96.834	15.531	52.289	1.00	19.99			N
ANISOU17843	N	LEU	D	267	2576	2484	2534	12	23	71		N
ATOM 17845	CA	LEU	D	267	96.067	16.442	53.104	1.00	19.90			C
ANISOU17845	CA	LEU	D	267	2522	2537	2501	-16	25	27		C
ATOM 17847	CB	LEU	D	267	94.593	16.385	52.739	1.00	19.42			C
ANISOU17847	CB	LEU	D	267	2472	2431	2475	-61	4	53		C
ATOM 17850	CG	LEU	D	267	93.658	17.235	53.607	1.00	19.49			C
ANISOU17850	CG	LEU	D	267	2454	2522	2429	-28	22	31		C
ATOM 17852	CD1	LEU	D	267	94.029	18.705	53.590	1.00	21.17			C
ANISOU17852	CD1	LEU	D	267	2534	2764	2743	-73	-9	-85		C
ATOM 17856	CD2	LEU	D	267	92.196	17.109	53.157	1.00	19.91			C
ANISOU17856	CD2	LEU	D	267	2471	2624	2470	-116	21	14		C
ATOM 17860	C	LEU	D	267	96.257	16.073	54.562	1.00	20.17			C
ANISOU17860	C	LEU	D	267	2508	2588	2565	15	-52	32		C
ATOM 17861	O	LEU	D	267	96.407	16.963	55.415	1.00	18.12			O
ANISOU17861	O	LEU	D	267	2094	2408	2381	44	-71	78		O
ATOM 17862	N	GLU	D	268	96.236	14.765	54.844	1.00	21.71			N
ANISOU17862	N	GLU	D	268	2704	2758	2784	-16	-32	6		N
ATOM 17903	CB	LEU	D	270	98.474	19.596	54.909	1.00	19.21			C
ANISOU17903	CB	LEU	D	270	2427	2467	2403	-43	89	13		C
ATOM 17906	CG	LEU	D	270	99.194	19.549	53.596	1.00	17.11			C
ANISOU17906	CG	LEU	D	270	2144	2233	2123	50	-68	20		C
ATOM 17908	CD1	LEU	D	270	98.227	20.120	52.556	1.00	13.24			C
ANISOU17908	CD1	LEU	D	270	1475	1738	1816	53	97	-84		C
ATOM 17922	CB	ALA	D	271	95.437	17.753	58.922	1.00	24.84			C
ANISOU17922	CB	ALA	D	271	3193	3201	3043	3	6	-22		C
ATOM 17961	CD1	LEU	D	274	97.816	23.568	58.951	1.00	36.84			C
ANISOU17961	CD1	LEU	D	274	4675	4670	4653	0	-6	-38		C
ATOM 18022	C	GLY	D	278	91.060	24.419	63.113	1.00	27.25			C
ANISOU18022	C	GLY	D	278	3456	3517	3379	-79	89	-9		C
ATOM 18023	O	GLY	D	278	90.308	23.665	62.458	1.00	27.42			O
ANISOU18023	O	GLY	D	278	3486	3598	3331	-191	168	50		O

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ATOM  18024  N   TYR D 279      92.119  25.047  62.606  1.00 25.34           N
ANISOU18024  N   TYR D 279    3287   3232   3106   -104     73      3       N
ATOM  18026  CA  TYR D 279      92.493  24.936  61.183  1.00 24.21           C
ANISOU18026  CA  TYR D 279    3097   3090   3008    -94     68     -7       C
ATOM  18028  CB  TYR D 279      93.631  25.928  60.822  1.00 23.42           C
ANISOU18028  CB  TYR D 279    2962   3033   2905   -120     56     15       C
ATOM  18031  CG  TYR D 279      93.758  26.251  59.321  1.00 22.60           C
ANISOU18031  CG  TYR D 279    2924   2826   2837    -46      0    -54       C
ATOM  18032  CD1 TYR D 279      93.176  27.388  58.790  1.00 21.78           C
ANISOU18032  CD1 TYR D 279    2871   2826   2578      3    -31   -117       C
ATOM  18034  CE1 TYR D 279      93.295  27.712  57.459  1.00 20.17           C
ANISOU18034  CE1 TYR D 279    2702   2457   2505    -97    122    -42       C
ATOM  18036  CZ  TYR D 279      94.055  26.880  56.603  1.00 17.34           C
ANISOU18036  CZ  TYR D 279    1973   2258   2358   -167      2    -39       C
ATOM  18037  OH  TYR D 279      94.191  27.182  55.253  1.00 14.53           O
ANISOU18037  OH  TYR D 279    1794   1673   2053   -160   -143   -367       O
ATOM  18039  CE2 TYR D 279      94.655  25.768  57.104  1.00 19.45           C
ANISOU18039  CE2 TYR D 279    2526   2327   2537    -98     66     47       C
ATOM  18041  CD2 TYR D 279      94.533  25.465  58.474  1.00 22.47           C
ANISOU18041  CD2 TYR D 279    3056   2856   2624    -56    -28    -30       C
ATOM  18043  C   TYR D 279      92.874  23.501  60.824  1.00 22.57           C
ANISOU18043  C   TYR D 279    2837   2942   2793    -94     76     30       C
ATOM  18044  O   TYR D 279      92.346  22.952  59.875  1.00 21.48           O
ANISOU18044  O   TYR D 279    2587   2926   2649   -306    280     21       O
ATOM  18045  N   GLY D 280      93.809  22.911  61.546  1.00 22.41           N
ANISOU18045  N   GLY D 280    2822   2920   2770    -82     35    -46       N
ATOM  18047  CA  GLY D 280      94.171  21.525  61.333  1.00 20.97           C
ANISOU18047  CA  GLY D 280    2566   2733   2668    -30    -16      3       C
ATOM  18050  C   GLY D 280      92.992  20.603  61.586  1.00 20.99           C
ANISOU18050  C   GLY D 280    2610   2723   2640      5      4    -26       C
ATOM  18051  O   GLY D 280      92.772  19.640  60.872  1.00 20.50           O
ANISOU18051  O   GLY D 280    2402   2686   2698    -82    -66   -127       O
ATOM  18067  C   GLN D 281      90.114  20.092  61.670  1.00 19.09           C
ANISOU18067  C   GLN D 281    2479   2375   2400      8    -37     37       C
ATOM  18068  O   GLN D 281      89.514  19.113  61.303  1.00 17.44           O
ANISOU18068  O   GLN D 281    2295   2157   2172     58    -66    155       O
ATOM  18069  N   TYR D 282      90.015  21.273  61.048  1.00 18.95           N
ANISOU18069  N   TYR D 282    2487   2323   2390    -18    -42     66       N
ATOM  18071  CA  TYR D 282      89.141  21.440  59.888  1.00 18.11           C
ANISOU18071  CA  TYR D 282    2427   2151   2299    -14    -53     59       C
ATOM  18073  CB  TYR D 282      89.100  22.904  59.461  1.00 18.63           C
ANISOU18073  CB  TYR D 282    2496   2275   2305    -29    -24     39       C
ATOM  18076  CG  TYR D 282      88.325  23.159  58.216  1.00 16.47           C
ANISOU18076  CG  TYR D 282    2127   2014   2115    -27     13    -49       C
ATOM  18077  CD1 TYR D 282      86.975  23.081  58.203  1.00 13.75           C
ANISOU18077  CD1 TYR D 282    1855   1609   1760     15    129      7       C
ATOM  18079  CE1 TYR D 282      86.269  23.346  57.070  1.00 14.20           C
ANISOU18079  CE1 TYR D 282    1953   1719   1721     93     85   -115       C
ATOM  18081  CZ  TYR D 282      86.908  23.699  55.912  1.00 12.49           C
ANISOU18081  CZ  TYR D 282    1726   1330   1689    -169     86     -1       C
ATOM  18082  OH  TYR D 282      86.155  23.976  54.769  1.00 12.84           O
ANISOU18082  OH  TYR D 282    1802   1358   1716    -151    180    -91       O
ATOM  18084  CE2 TYR D 282      88.248  23.800  55.902  1.00 15.47           C
ANISOU18084  CE2 TYR D 282    2068   1804   2006     62    -46    -57       C
ATOM  18086  CD2 TYR D 282      88.962  23.532  57.038  1.00 16.57           C
ANISOU18086  CD2 TYR D 282    2090   2172   2031   -120    -12     47       C
ATOM  18088  C   TYR D 282      89.607  20.570  58.714  1.00 17.79           C
ANISOU18088  C   TYR D 282    2355   2117   2285    -16    -36     71       C
ATOM  18089  O   TYR D 282      88.804  19.857  58.097  1.00 17.64           O
ANISOU18089  O   TYR D 282    2316   2150   2237      1   -253     87       O
ATOM  18090  N   LEU D 283      90.889  20.632  58.400  1.00 17.34           N
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ANISOU18090	N	LEU	D	283	2348	2022	2216	21	-81	82				N
ATOM	18092	CA	LEU	D	283	91.456	19.815	57.342	1.00	17.75				C
ANISOU18092	CA	LEU	D	283	2308	2186	2248	5	-15	59				C
ATOM	18094	CB	LEU	D	283	92.949	20.073	57.252	1.00	18.08				C
ANISOU18094	CB	LEU	D	283	2343	2214	2310	-15	-18	52				C
ATOM	18097	CG	LEU	D	283	93.257	21.545	56.902	1.00	19.25				C
ANISOU18097	CG	LEU	D	283	2431	2378	2506	36	-31	-6				C
ATOM	18099	CD1	LEU	D	283	94.683	21.736	56.613	1.00	20.03				C
ANISOU18099	CD1	LEU	D	283	2704	2451	2452	-156	252	-20				C
ATOM	18103	CD2	LEU	D	283	92.386	21.975	55.758	1.00	20.46				C
ANISOU18103	CD2	LEU	D	283	2868	2539	2365	-40	91	27				C
ATOM	18107	C	LEU	D	283	91.194	18.335	57.583	1.00	18.19				C
ANISOU18107	C	LEU	D	283	2334	2239	2335	14	-10	-6				C
ATOM	18108	O	LEU	D	283	90.792	17.614	56.672	1.00	18.11				O
ANISOU18108	O	LEU	D	283	2249	2257	2373	22	-86	-11				O
ATOM	18109	N	LYS	D	284	91.412	17.882	58.813	1.00	18.90				N
ANISOU18109	N	LYS	D	284	2436	2358	2384	-11	-56	-52				N
ATOM	18111	CA	LYS	D	284	91.168	16.483	59.148	1.00	19.62				C
ANISOU18111	CA	LYS	D	284	2500	2474	2480	-15	-21	46				C
ATOM	18129	C	LYS	D	284	89.711	16.096	58.853	1.00	18.87				C
ANISOU18129	C	LYS	D	284	2408	2416	2343	-23	-5	97				C
ATOM	18130	O	LYS	D	284	89.434	15.041	58.326	1.00	18.01				O
ANISOU18130	O	LYS	D	284	2157	2408	2275	-56	-183	209				O
ATOM	18131	N	ARG	D	285	88.795	16.972	59.157	1.00	19.11				N
ANISOU18131	N	ARG	D	285	2455	2414	2389	-68	29	142				N
ATOM	18133	CA	ARG	D	285	87.371	16.667	58.959	1.00	20.61				C
ANISOU18133	CA	ARG	D	285	2598	2582	2649	-34	-54	78				C
ATOM	18135	CB	ARG	D	285	86.549	17.732	59.630	1.00	20.85				C
ANISOU18135	CB	ARG	D	285	2642	2644	2635	-66	27	116				C
ATOM	18138	CG	ARG	D	285	85.138	17.618	59.292	1.00	25.19				C
ANISOU18138	CG	ARG	D	285	3069	3231	3269	-45	-153	97				C
ATOM	18141	CD	ARG	D	285	84.180	18.252	60.283	1.00	30.00				C
ANISOU18141	CD	ARG	D	285	3779	3893	3724	-27	144	-66				C
ATOM	18144	NE	ARG	D	285	84.349	19.686	60.519	1.00	34.32				N
ANISOU18144	NE	ARG	D	285	4520	4113	4407	-3	25	23				N
ATOM	18146	CZ	ARG	D	285	83.705	20.659	59.857	1.00	34.86				C
ANISOU18146	CZ	ARG	D	285	4439	4306	4499	74	-57	9				C
ATOM	18147	NH1	ARG	D	285	82.860	20.373	58.857	1.00	36.54				N
ANISOU18147	NH1	ARG	D	285	4712	4548	4623	8	-96	-70				N
ATOM	18150	NH2	ARG	D	285	83.930	21.922	60.196	1.00	32.17				N
ANISOU18150	NH2	ARG	D	285	4010	4047	4165	46	18	93				N
ATOM	18153	C	ARG	D	285	86.964	16.490	57.486	1.00	20.79				C
ANISOU18153	C	ARG	D	285	2599	2589	2711	1	-64	84				C
ATOM	18154	O	ARG	D	285	86.068	15.697	57.138	1.00	20.29				O
ANISOU18154	O	ARG	D	285	2554	2412	2743	17	-124	226				O
ATOM	18155	N	LEU	D	286	87.619	17.237	56.617	1.00	21.21				N
ANISOU18155	N	LEU	D	286	2578	2699	2778	7	-3	46				N
ATOM	18157	CA	LEU	D	286	87.355	17.160	55.198	1.00	22.40				C
ANISOU18157	CA	LEU	D	286	2755	2893	2862	9	-48	14				C
ATOM	18159	CB	LEU	D	286	88.129	18.232	54.469	1.00	23.39				C
ANISOU18159	CB	LEU	D	286	2962	3021	2901	-26	-58	43				C
ATOM	18162	CG	LEU	D	286	87.681	19.636	54.863	1.00	25.94				C
ANISOU18162	CG	LEU	D	286	3348	3313	3194	33	-13	-44				C
ATOM	18164	CD1	LEU	D	286	88.501	20.677	54.176	1.00	28.20				C
ANISOU18164	CD1	LEU	D	286	3695	3574	3442	-69	117	-3				C
ATOM	18168	CD2	LEU	D	286	86.203	19.889	54.562	1.00	28.64				C
ANISOU18168	CD2	LEU	D	286	3530	3777	3573	22	-24	-16				C
ATOM	18172	C	LEU	D	286	87.696	15.808	54.610	1.00	22.57				C
ANISOU18172	C	LEU	D	286	2832	2849	2894	-50	-49	55				C
ATOM	18173	O	LEU	D	286	87.313	15.491	53.464	1.00	22.32				O
ANISOU18173	O	LEU	D	286	2816	2811	2850	-59	-179	190				O

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ATOM  18174  N   LEU D 287      88.452  15.010  55.359  1.00 22.09           N
ANISOU18174  N   LEU D 287     2744   2842   2806    -63    -72      63      N
ATOM  18176  CA  LEU D 287      88.773  13.681  54.898  1.00 22.67           C
ANISOU18176  CA  LEU D 287     2839   2889   2883    -13    -39      46      C
ATOM  18178  CB  LEU D 287      89.993  13.094  55.628  1.00 22.85           C
ANISOU18178  CB  LEU D 287     2807   2982   2893    -29    -39      10      C
ATOM  18181  CG  LEU D 287      91.373  13.739  55.405  1.00 24.06           C
ANISOU18181  CG  LEU D 287     3050   3066   3022    -28     54      13      C
ATOM  18183  CD1 LEU D 287      92.298  13.241  56.508  1.00 25.08           C
ANISOU18183  CD1 LEU D 287     3085   3226   3217     23     -2     -92      C
ATOM  18187  CD2 LEU D 287      91.958  13.463  54.022  1.00 23.08           C
ANISOU18187  CD2 LEU D 287     3004   2752   3012     42     65     -33      C
ATOM  18191  C   LEU D 287      87.601  12.727  55.102  1.00 22.23           C
ANISOU18191  C   LEU D 287     2758   2830   2854    -18   -115      33      C
ATOM  18192  O   LEU D 287      87.513  11.753  54.355  1.00 23.01           O
ANISOU18192  O   LEU D 287     2829   2751   3159      0   -225      72      O
ATOM  18193  N   THR D 288      86.759  13.000  56.103  1.00 21.67           N
ANISOU18193  N   THR D 288     2648   2721   2862     25    -94      72      N
ATOM  18195  CA  THR D 288      85.638  12.117  56.519  1.00 22.58           C
ANISOU18195  CA  THR D 288     2735   2881   2961     33    -39      44      C
ATOM  18205  C   THR D 288      84.226  12.700  56.347  1.00 21.40           C
ANISOU18205  C   THR D 288     2644   2710   2777     29      3      69      C
ATOM  18207  N   GLU D 289      84.105  13.745  55.558  1.00 19.74           N
ANISOU18207  N   GLU D 289     2473   2502   2525     12    -51     -33      N
ATOM  18209  CA  GLU D 289      82.828  14.362  55.343  1.00 17.87           C
ANISOU18209  CA  GLU D 289     2272   2231   2287     38     34     -28      C
ATOM  18211  CB  GLU D 289      82.766  15.696  56.107  1.00 18.82           C
ANISOU18211  CB  GLU D 289     2390   2431   2330     26      2     -71      C
ATOM  18214  CG  GLU D 289      81.337  16.241  56.183  1.00 18.36           C
ANISOU18214  CG  GLU D 289     2264   2363   2347     97    -24      14      C
ATOM  18217  CD  GLU D 289      81.227  17.667  56.736  1.00 21.02           C
ANISOU18217  CD  GLU D 289     2657   2548   2782     14     67    -123      C
ATOM  18218  OE1 GLU D 289      82.274  18.358  56.890  1.00 21.45           O
ANISOU18218  OE1 GLU D 289     2894   2412   2844     60     27    -240      O
ATOM  18219  OE2 GLU D 289      80.077  18.072  57.035  1.00 20.60           O
ANISOU18219  OE2 GLU D 289     2730   2234   2862    267   -193     -62      O
ATOM  18220  C   GLU D 289      82.649  14.675  53.875  1.00 16.22           C
ANISOU18220  C   GLU D 289     2045   2026   2092     60     31     -67      C
ATOM  18221  O   GLU D 289      83.540  15.259  53.285  1.00 17.47           O
ANISOU18221  O   GLU D 289     2238   2379   2018    136    117     -36      O
ATOM  18222  N   THR D 290      81.483  14.377  53.311  1.00 14.59           N
ANISOU18222  N   THR D 290     2002   1752   1787     75     63     -80      N
ATOM  18224  CA  THR D 290      81.146  14.822  51.957  1.00 13.30           C
ANISOU18224  CA  THR D 290     1647   1658   1746     75    -14     -51      C
ATOM  18226  CB  THR D 290      80.161  13.848  51.295  1.00 14.18           C
ANISOU18226  CB  THR D 290     1765   1796   1825     82    -59     -42      C
ATOM  18228  OG1 THR D 290      80.799  12.597  51.037  1.00 17.72           O
ANISOU18228  OG1 THR D 290     2105   2207   2419    218   -134     -90      O
ATOM  18230  CG2 THR D 290      79.717  14.347  49.896  1.00 12.57           C
ANISOU18230  CG2 THR D 290     1738   1468   1571     14    -52     -140      C
ATOM  18234  C   THR D 290      80.562  16.236  52.014  1.00 11.49           C
ANISOU18234  C   THR D 290     1395   1542   1426     27    -72      35      C
ATOM  18235  O   THR D 290      79.590  16.506  52.708  1.00 11.72           O
ANISOU18235  O   THR D 290     1425   1606   1421     98    -79       8      O
ATOM  18236  N   VAL D 291      81.150  17.146  51.287  1.00 10.13           N
ANISOU18236  N   VAL D 291     1134   1369   1345     49     -2     -13      N
ATOM  18238  CA  VAL D 291      80.644  18.529  51.242  1.00  9.71           C
ANISOU18238  CA  VAL D 291     1100   1329   1257     53     55      -1      C
ATOM  18240  CB  VAL D 291      81.703  19.569  51.742  1.00  9.58           C
ANISOU18240  CB  VAL D 291     1141   1260   1238    -17    107      22      C
ATOM  18242  CG1 VAL D 291      81.217  20.975  51.614  1.00  8.64           C
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ANISOU18242	CG1	VAL	D	291	836	1313	1133	78	-53	-33		C
ATOM 18246	CG2	VAL	D	291	82.095	19.345	53.170	1.00	11.02			C
ANISOU18246	CG2	VAL	D	291	1128	1557	1501	107	-119	114		C
ATOM 18250	C	VAL	D	291	80.279	18.802	49.801	1.00	9.92			C
ANISOU18250	C	VAL	D	291	1203	1354	1211	50	99	-42		C
ATOM 18251	O	VAL	D	291	81.154	18.725	48.913	1.00	10.32			O
ANISOU18251	O	VAL	D	291	1203	1531	1185	248	236	-49		O
ATOM 18252	N	TYR	D	292	79.017	19.143	49.573	1.00	9.62			N
ANISOU18252	N	TYR	D	292	1168	1316	1169	104	113	-82		N
ATOM 18254	CA	TYR	D	292	78.475	19.404	48.268	1.00	11.45			C
ANISOU18254	CA	TYR	D	292	1482	1464	1406	44	42	-28		C
ATOM 18256	CB	TYR	D	292	76.973	19.151	48.270	1.00	10.83			C
ANISOU18256	CB	TYR	D	292	1432	1373	1307	52	15	-49		C
ATOM 18259	CG	TYR	D	292	76.646	17.772	48.695	1.00	9.96			C
ANISOU18259	CG	TYR	D	292	1181	1427	1175	201	-118	145		C
ATOM 18260	CD1	TYR	D	292	75.959	17.543	49.874	1.00	8.91			C
ANISOU18260	CD1	TYR	D	292	889	1317	1177	231	-81	171		C
ATOM 18262	CE1	TYR	D	292	75.687	16.273	50.262	1.00	11.78			C
ANISOU18262	CE1	TYR	D	292	1526	1419	1530	79	70	128		C
ATOM 18264	CZ	TYR	D	292	76.016	15.181	49.462	1.00	11.39			C
ANISOU18264	CZ	TYR	D	292	1326	1522	1478	76	85	56		C
ATOM 18265	OH	TYR	D	292	75.731	13.914	49.954	1.00	13.39			O
ANISOU18265	OH	TYR	D	292	1607	1473	2007	101	-64	-61		O
ATOM 18267	CE2	TYR	D	292	76.678	15.369	48.297	1.00	12.20			C
ANISOU18267	CE2	TYR	D	292	1721	1559	1355	81	-3	71		C
ATOM 18269	CD2	TYR	D	292	76.988	16.684	47.904	1.00	10.05			C
ANISOU18269	CD2	TYR	D	292	1216	1386	1214	115	-10	-21		C
ATOM 18271	C	TYR	D	292	78.728	20.820	47.802	1.00	13.53			C
ANISOU18271	C	TYR	D	292	1873	1610	1657	91	12	12		C
ATOM 18272	O	TYR	D	292	78.566	21.015	46.594	1.00	15.36			O
ANISOU18272	O	TYR	D	292	2248	1872	1713	176	202	79		O
ATOM 18273	OXT	TYR	D	292	79.058	21.621	48.661	1.00	15.02			O
ANISOU18273	OXT	TYR	D	292	2059	1782	1863	34	-29	0		O
ATOM 20579	CA	ASP	E	150	63.835	16.845	36.379	1.00	19.75			C
ANISOU20579	CA	ASP	E	150	2540	2527	2437	3	-14	6		C
ATOM 20581	CB	ASP	E	150	63.521	16.810	37.882	1.00	20.77			C
ANISOU20581	CB	ASP	E	150	2749	2620	2521	70	79	-40		C
ATOM 20584	CG	ASP	E	150	63.222	15.432	38.415	1.00	22.96			C
ANISOU20584	CG	ASP	E	150	3132	2829	2761	26	86	51		C
ATOM 20586	OD2	ASP	E	150	62.722	15.336	39.552	1.00	25.38			O
ANISOU20586	OD2	ASP	E	150	3636	3229	2775	127	317	-44		O
ATOM 20587	C	ASP	E	150	64.974	15.900	36.017	1.00	20.35			C
ANISOU20587	C	ASP	E	150	2568	2657	2504	23	45	-20		C
ATOM 20589	N	GLN	E	151	66.107	16.073	36.678	1.00	20.64			N
ANISOU20589	N	GLN	E	151	2648	2777	2417	-32	-52	10		N
ATOM 20591	CA	GLN	E	151	67.290	15.291	36.326	1.00	23.23			C
ANISOU20591	CA	GLN	E	151	2962	2987	2875	56	-32	-9		C
ATOM 20593	CB	GLN	E	151	68.504	15.758	37.101	1.00	23.58			C
ANISOU20593	CB	GLN	E	151	2919	3098	2943	-42	16	62		C
ATOM 20596	CG	GLN	E	151	68.711	17.163	36.846	1.00	28.43			C
ANISOU20596	CG	GLN	E	151	3741	3461	3599	30	-11	-20		C
ATOM 20599	CD	GLN	E	151	70.085	17.584	37.124	1.00	33.30			C
ANISOU20599	CD	GLN	E	151	3986	4277	4387	-132	-1	43		C
ATOM 20600	OE1	GLN	E	151	71.014	16.757	37.168	1.00	36.56			O
ANISOU20600	OE1	GLN	E	151	4755	4289	4848	64	2	78		O
ATOM 20601	NE2	GLN	E	151	70.257	18.885	37.324	1.00	37.87			N
ANISOU20601	NE2	GLN	E	151	4946	4495	4947	32	-30	4		N
ATOM 20604	C	GLN	E	151	67.102	13.822	36.530	1.00	23.67			C
ANISOU20604	C	GLN	E	151	2983	3057	2952	33	-25	29		C
ATOM 20605	O	GLN	E	151	67.744	12.989	35.856	1.00	25.73			O
ANISOU20605	O	GLN	E	151	3298	3266	3213	198	23	-17		O

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ATOM  20606  N   GLY E 152      66.210  13.483  37.432  1.00 23.38           N
ANISOU20606  N   GLY E 152    2949   3023   2911     89    -43     -7       N
ATOM  36741  C1, TDG M 600      69.071  40.140  46.254  1.00 12.52           C
ANISOU36741  C1, TDG M 600    1652   1528   1577    -43    -40     48       C
ATOM  36743  C2, TDG M 600      68.642  38.804  45.927  1.00 12.49           C
ANISOU36743  C2, TDG M 600    1848   1479   1417    119   -135     46       C
ATOM  36746  O4, TDG M 600      70.367  40.187  45.700  1.00 12.98           O
ANISOU36746  O4, TDG M 600    1631   1743   1557    -35   -110     31       O
ATOM  36747  C4, TDG M 600      70.895  38.888  45.554  1.00 12.38           C
ANISOU36747  C4, TDG M 600    1599   1681   1422    -47     31     68       C
ATOM  36749  C3, TDG M 600      69.814  37.853  45.978  1.00 11.39           C
ANISOU36749  C3, TDG M 600    1283   1383   1661   -210    -54      6       C
ATOM  36751  O3, TDG M 600      70.084  37.467  47.319  1.00 13.06           O
ANISOU36751  O3, TDG M 600    1517   1915   1528    101     89     66       O
ATOM  36753  C5, TDG M 600      71.471  38.716  44.170  1.00 10.61           C
ANISOU36753  C5, TDG M 600    1263   1301   1468   -252     -2    231       C
ATOM  36756  O5, TDG M 600      70.401  38.888  43.273  1.00 11.41           O
ANISOU36756  O5, TDG M 600    1494   1490   1351    116     32    379       O
ATOM  36757  P   TDG M 600      70.149  37.834  42.076  1.00 12.32           P
ANISOU36757  P   TDG M 600    1732   1567   1380    122    122    152       P
ATOM  36758  O1P TDG M 600      69.289  38.482  40.969  1.00 14.76           O
ANISOU36758  O1P TDG M 600    1613   2073   1919     33   -276    224       O
ATOM  36759  O2P TDG M 600      69.742  36.452  42.561  1.00 12.62           O
ANISOU36759  O2P TDG M 600    1535   1558   1699   -136     71    123       O
ATOM  36760  OPP TDG M 600      71.627  37.565  41.456  1.00 12.91           O
ANISOU36760  OPP TDG M 600    1878   1484   1543      0    238    219       O
ATOM  36761  P2  TDG M 600      72.743  38.612  40.959  1.00 12.98           P
ANISOU36761  P2  TDG M 600    1503   1763   1663   -113    251    -83       P
ATOM  36762  O3P TDG M 600      74.118  38.290  41.621  1.00 14.23           O
ANISOU36762  O3P TDG M 600    1998   1597   1812     16    138    133       O
ATOM  36763  O4P TDG M 600      72.259  40.106  40.978  1.00 14.72           O
ANISOU36763  O4P TDG M 600    2204   1690   1699    -71    320    553       O
ATOM  36764  O1  TDG M 600      72.876  38.100  39.426  1.00 12.82           O
ANISOU36764  O1  TDG M 600    1910   1383   1577    -94      0    233       O
ATOM  36765  C1  TDG M 600      72.000  38.634  38.397  1.00 13.50           C
ANISOU36765  C1  TDG M 600    1534   1903   1692    -41   -259     68       C
ATOM  36767  C2  TDG M 600      71.560  37.546  37.444  1.00 14.62           C
ANISOU36767  C2  TDG M 600    1975   1745   1836     58   -112     40       C
ATOM  36769  O2  TDG M 600      70.988  36.403  38.131  1.00 18.41           O
ANISOU36769  O2  TDG M 600    2442   2521   2032   -394    203    -72       O
ATOM  36771  C3  TDG M 600      72.716  37.132  36.563  1.00 13.69           C
ANISOU36771  C3  TDG M 600    1492   1916   1792     82    -86    -16       C
ATOM  36773  O3  TDG M 600      72.247  36.256  35.535  1.00 16.32           O
ANISOU36773  O3  TDG M 600    1480   2450   2270    294    -62    -18       O
ATOM  36775  C4  TDG M 600      73.471  38.309  35.953  1.00 16.71           C
ANISOU36775  C4  TDG M 600    2150   2149   2048     12     34     30       C
ATOM  36777  O4  TDG M 600      74.652  37.783  35.244  1.00 16.79           O
ANISOU36777  O4  TDG M 600    2094   2001   2283   -101    122    -37       O
ATOM  36779  C5  TDG M 600      73.968  39.273  37.062  1.00 17.56           C
ANISOU36779  C5  TDG M 600    2392   2141   2139    -70     54     -1       C
ATOM  36781  O5  TDG M 600      72.923  39.661  37.942  1.00 15.41           O
ANISOU36781  O5  TDG M 600    2084   1974   1797   -178   -205     82       O
ATOM  36967  O41 TDG Q 600      86.862  24.808  48.956  1.00 16.34           O
ANISOU36967  O41 TDG Q 600    2009   1872   2327     45    256    262       O
ATOM  36968  C41 TDG Q 600      86.276  25.942  48.639  1.00 16.13           C
ANISOU36968  C41 TDG Q 600    1640   2189   2299     46    218     30       C
ATOM  36969  N31 TDG Q 600      86.639  27.024  49.319  1.00 17.72           N
ANISOU36969  N31 TDG Q 600    2177   2254   2303     47    101    121       N
ATOM  36971  C21 TDG Q 600      86.068  28.205  49.065  1.00 17.09           C
ANISOU36971  C21 TDG Q 600    1981   2256   2254    174    -22    -93       C
ATOM  36972  O21 TDG Q 600      86.490  29.234  49.737  1.00 17.42           O
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ANISOU36972  O21 TDG Q 600     1931   2032   2656    169   -225     67       O
ATOM  36973  C51 TDG Q 600      85.288  26.008  47.681  1.00 16.19           C
ANISOU36973  C51 TDG Q 600     2079   2108   1962    -32    163     78       C
ATOM  36974  C5A TDG Q 600      84.884  24.753  46.957  1.00 19.08           C
ANISOU36974  C5A TDG Q 600     2282   2282   2682     11    -11     36       C
ATOM  36978  C61 TDG Q 600      84.680  27.239  47.456  1.00 15.21           C
ANISOU36978  C61 TDG Q 600     1540   2281   1957     57    -80    -16       C
ATOM  36980  N11 TDG Q 600      85.096  28.329  48.129  1.00 14.21           N
ANISOU36980  N11 TDG Q 600     1665   1752   1981    123     50     68       N
ATOM  36981  C1, TDG Q 600      84.476  29.626  47.985  1.00 12.97           C
ANISOU36981  C1, TDG Q 600     1608   1754   1564     64    -35    -22       C
ATOM  36983  C2, TDG Q 600      84.517  29.998  46.571  1.00 10.65           C
ANISOU36983  C2, TDG Q 600     1207   1271   1569     49    155    188       C
ATOM  36986  O4, TDG Q 600      83.070  29.500  48.222  1.00 15.58           O
ANISOU36986  O4, TDG Q 600     2004   1706   2210     69     92    176       O
ATOM  36987  C4, TDG Q 600      82.335  30.200  47.183  1.00 10.85           C
ANISOU36987  C4, TDG Q 600     1307   1505   1307    -52    194   -107       C
ATOM  36989  C3, TDG Q 600      83.333  30.876  46.174  1.00 10.14           C
ANISOU36989  C3, TDG Q 600     1002   1414   1435   -142    114    134       C
ATOM  36991  O3, TDG Q 600      83.442  32.199  46.606  1.00 12.71           O
ANISOU36991  O3, TDG Q 600     1015   1589   2223     71    320    -98       O
ATOM  36993  C5, TDG Q 600      81.323  29.283  46.569  1.00 11.47           C
ANISOU36993  C5, TDG Q 600     1290   1667   1398    334   -350    396       C
ATOM  36996  O5, TDG Q 600      81.940  28.227  45.894  1.00 14.18           O
ANISOU36996  O5, TDG Q 600     1581   1785   2022   -282     91     -1       O
ATOM  36997  P   TDG Q 600      81.448  27.903  44.409  1.00 16.76           P
ANISOU36997  P   TDG Q 600     1786   2425   2154    -17     19    101       P
ATOM  36998  O1P TDG Q 600      82.020  26.443  44.163  1.00 18.61           O
ANISOU36998  O1P TDG Q 600     2672   2271   2128     42    149    159       O
ATOM  36999  O2P TDG Q 600      81.711  29.039  43.369  1.00 17.08           O
ANISOU36999  O2P TDG Q 600     2134   1997   2359   -108    -77   -137       O
ATOM  37000  OPP TDG Q 600      79.802  27.834  44.549  1.00 13.41           O
ANISOU37000  OPP TDG Q 600     1535   1777   1783    124    -55     32       O
ATOM  37001  P2  TDG Q 600      78.855  27.029  45.563  1.00 15.84           P
ANISOU37001  P2  TDG Q 600     2054   2158   1805     96   -199    -11       P
ATOM  37002  O3P TDG Q 600      77.787  28.041  46.105  1.00 13.69           O
ANISOU37002  O3P TDG Q 600     1685   1849   1667   -127   -195     88       O
ATOM  37003  O4P TDG Q 600      79.656  26.000  46.445  1.00 18.24           O
ANISOU37003  O4P TDG Q 600     2327   2364   2237    115   -245     18       O
ATOM  37004  O1  TDG Q 600      78.002  26.083  44.500  1.00 14.18           O
ANISOU37004  O1  TDG Q 600     1916   1811   1659    -94     -4    265       O
ATOM  37005  C1  TDG Q 600      78.429  24.770  44.050  1.00 16.67           C
ANISOU37005  C1  TDG Q 600     2129   1958   2245     59     81    -80       C
ATOM  37007  C2  TDG Q 600      78.121  24.558  42.619  1.00 18.04           C
ANISOU37007  C2  TDG Q 600     2317   2135   2402     20    -13     47       C
ATOM  37009  O2  TDG Q 600      78.792  25.524  41.827  1.00 19.74           O
ANISOU37009  O2  TDG Q 600     2413   2320   2765   -162     53    -41       O
ATOM  37011  C3  TDG Q 600      76.604  24.563  42.375  1.00 17.10           C
ANISOU37011  C3  TDG Q 600     2163   2060   2272    -52     46    -34       C
ATOM  37013  O3  TDG Q 600      76.444  24.130  41.027  1.00 16.67           O
ANISOU37013  O3  TDG Q 600     1910   2067   2354    -46    -23     26       O
ATOM  37015  C4  TDG Q 600      75.983  23.542  43.320  1.00 17.79           C
ANISOU37015  C4  TDG Q 600     2378   2019   2360    123     70     82       C
ATOM  37017  O4  TDG Q 600      74.571  23.410  43.131  1.00 20.12           O
ANISOU37017  O4  TDG Q 600     2672   2103   2867   -362    -46     10       O
ATOM  37019  C5  TDG Q 600      76.263  23.940  44.759  1.00 18.99           C
ANISOU37019  C5  TDG Q 600     2496   2241   2477    -59      1    135       C
ATOM  37021  O5  TDG Q 600      77.649  24.013  44.971  1.00 18.79           O
ANISOU37021  O5  TDG Q 600     2468   2220   2448    -55    206    -98       O
ATOM  37022  C6  TDG Q 600      75.801  22.898  45.774  1.00 18.41           C
ANISOU37022  C6  TDG Q 600     2330   2269   2396     72    237     62       C
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ATOM  37025  O6  TDG Q 600      76.267  21.596  45.472  1.00 17.18           O
ANISOU37025  O6  TDG Q 600    2665   1570   2292   -282    186    104       O
ATOM  37548  S   SO4 J   1     72.371  26.539  41.932  1.00 43.95           S
ANISOU37548  S   SO4 J   1    5527   5558   5611    -21   -109     13       S
ATOM  37549  O1  SO4 J   1     73.643  25.829  42.171  1.00 40.90           O
ANISOU37549  O1  SO4 J   1    5221   4857   5461    -37    -94   -162       O
ATOM  37550  O2  SO4 J   1     72.568  27.564  40.840  1.00 42.62           O
ANISOU37550  O2  SO4 J   1    5535   5405   5252      1    -10     15       O
ATOM  37551  O3  SO4 J   1     71.309  25.587  41.707  1.00 41.68           O
ANISOU37551  O3  SO4 J   1    5399   5239   5198    -65   -230    -11       O
ATOM  37552  O4  SO4 J   1     71.974  27.257  43.160  1.00 42.60           O
ANISOU37552  O4  SO4 J   1    5240   5559   5387     33    -10     13       O
ATOM  37581  O   HOH I   7     77.730  22.240  50.912  1.00 16.46           O
ANISOU37581  O   HOH I   7    2098   1901   2253    321    358    260       O
ATOM  37599  O   HOH I  13     87.886  42.778  36.972  1.00 14.12           O
ANISOU37599  O   HOH I  13    1727   1858   1779    693   -111   -101       O
ATOM  37614  O   HOH I  18     75.994  24.384  51.895  1.00 11.33           O
ANISOU37614  O   HOH I  18    1664   1593   1047   -215    167    -22       O
ATOM  37659  O   HOH I  33     76.692  34.694  46.646  1.00 11.31           O
ANISOU37659  O   HOH I  33    1421   1813   1061    144   -334      5       O
ATOM  37668  O   HOH I  36     76.863  26.212  53.757  1.00  9.98           O
ANISOU37668  O   HOH I  36    1199   1323   1268    -66    -33    170       O
ATOM  37701  O   HOH I  47     77.668  16.261  56.572  1.00 20.19           O
ANISOU37701  O   HOH I  47    2668   2473   2530    119     84    212       O
ATOM  37737  O   HOH I  59     73.167  25.841  45.314  1.00 13.31           O
ANISOU37737  O   HOH I  59    1662   2103   1291      6    178   -184       O
ATOM  37836  O   HOH I  92     63.163  21.494  43.620  1.00 15.08           O
ANISOU37836  O   HOH I  92    2002   1638   2088   -275    179    135       O
ATOM  37893  O   HOH I 111     68.277  37.809  49.089  1.00 14.09           O
ANISOU37893  O   HOH I 111    1653   2108   1591    -90   -116    320       O
ATOM  37896  O   HOH I 112     78.713  24.362  48.362  1.00 15.00           O
ANISOU37896  O   HOH I 112    1666   1943   2089     70    190    216       O
ATOM  37899  O   HOH I 113     77.609  45.126  43.459  1.00 11.10           O
ANISOU37899  O   HOH I 113    2133   1070   1014     -6    199    258       O
ATOM  37941  O   HOH I 127     85.710  45.011  53.303  1.00 17.31           O
ANISOU37941  O   HOH I 127    2409   2218   1948    107    -18    122       O
ATOM  38031  O   HOH I 157     74.336  12.788  54.780  1.00 17.23           O
ANISOU38031  O   HOH I 157    1791   2331   2422    478   -145   -180       O
ATOM  38037  O   HOH I 159     97.934  26.920  56.050  1.00 21.51           O
ANISOU38037  O   HOH I 159    2077   3012   3082   -232   -321    252       O
ATOM  38040  O   HOH I 160     83.513  16.448  49.990  1.00 21.25           O
ANISOU38040  O   HOH I 160    2658   2390   3022    328    215    248       O
ATOM  38055  O   HOH I 165     77.473  37.866  37.791  1.00 14.84           O
ANISOU38055  O   HOH I 165    1919   1734   1986    -76    -88     59       O
ATOM  38061  O   HOH I 167     88.096  26.769  51.687  1.00 13.74           O
ANISOU38061  O   HOH I 167    1133   2049   2038    109    106    333       O
ATOM  38064  O   HOH I 168     64.424  24.683  52.860  1.00 13.22           O
ANISOU38064  O   HOH I 168    1669   2056   1298    113     54   -362       O
ATOM  38121  O   HOH I 187     83.144  28.702  51.970  1.00 19.82           O
ANISOU38121  O   HOH I 187    2962   1996   2572    255   -597   -100       O
ATOM  38181  O   HOH I 207     88.691  35.310  48.169  1.00 20.46           O
ANISOU38181  O   HOH I 207    2073   3421   2278     58   -446     20       O
ATOM  38253  O   HOH I 231     85.979  33.047  47.066  1.00 16.89           O
ANISOU38253  O   HOH I 231    2094   1912   2408     54     23    -14       O
ATOM  38331  O   HOH I 257     64.201  23.448  41.992  1.00 20.24           O
ANISOU38331  O   HOH I 257    2311   2539   2840    198   -138     27       O
ATOM  38352  O   HOH I 264     81.992  22.886  48.432  1.00 17.31           O
ANISOU38352  O   HOH I 264    2606   2029   1940   -129    -99   -125       O
ATOM  38451  O   HOH I 297     65.761  15.182  46.292  1.00 22.59           O
ANISOU38451  O   HOH I 297    2699   2454   3430    -89   -154   -355       O
ATOM  38478  O   HOH I 306     65.697  25.417  43.115  1.00 19.42           O
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ANISOU38478  O   HOH I 306     2937   2136   2306    435    314   -132      O
ATOM  38529  O   HOH I 323      90.221  36.889  46.346  1.00 20.41           O
ANISOU38529  O   HOH I 323     2545   2561   2648    242    162    -55      O
ATOM  38832  O   HOH I 424      63.087  22.268  39.278  1.00 30.72           O
ANISOU38832  O   HOH I 424     3920   3965   3785    -47   -262   -127      O
ATOM  38919  O   HOH I 453      67.715  17.228  44.363  1.00 27.90           O
ANISOU38919  O   HOH I 453     3496   3862   3240   -373   -149   -234      O
ATOM  38934  O   HOH I 458      81.354  24.361  46.004  1.00 24.09           O
ANISOU38934  O   HOH I 458     3127   3187   2836    200   -243    -86      O
ATOM  38964  O   HOH I 468      73.471  33.889  35.812  1.00 24.60           O
ANISOU38964  O   HOH I 468     3640   2438   3268     95    225    -62      O
ATOM  38970  O   HOH I 470      76.522  33.034  37.156  1.00 29.47           O
ANISOU38970  O   HOH I 470     4063   3727   3407     29    107   -115      O
ATOM  39081  O   HOH I 507      71.335  20.178  44.538  1.00 23.63           O
ANISOU39081  O   HOH I 507     2776   3352   2848    -92    231   -295      O
ATOM  39195  O   HOH I 545      76.135  35.410  36.289  1.00 28.45           O
ANISOU39195  O   HOH I 545     3443   3957   3407      5    -43    513      O
ATOM  39252  O   HOH I 564      71.034  23.217  43.996  1.00 31.12           O
ANISOU39252  O   HOH I 564     4381   3738   3704   -191    153   -264      O
ATOM  39534  O   HOH I 658      79.531  12.996  54.737  1.00 23.78           O
ANISOU39534  O   HOH I 658     2826   2973   3237      4     20    327      O
ATOM  39546  O   HOH I 662      78.450  38.008  34.360  1.00 35.27           O
ANISOU39546  O   HOH I 662     4760   4563   4078   -312    155   -140      O
ATOM  39555  O   HOH I 665      65.184  29.767  37.286  1.00 26.86           O
ANISOU39555  O   HOH I 665     3320   3655   3230   -534    -36    138      O
ATOM  39600  O   HOH I 680      68.064  27.091  39.320  1.00 30.93           O
ANISOU39600  O   HOH I 680     3898   4393   3460    268   -136    -90      O
ATOM  39795  O   HOH I 745      65.311  17.380  42.990  0.00 29.76           O
ANISOU39795  O   HOH I 745     3657   3838   3814    -15    122     60      O
ATOM  39798  O   HOH I 746      73.979  20.306  44.028  1.00 33.29           O
ANISOU39798  O   HOH I 746     4033   4481   4134   -145    278   -264      O
ATOM  39810  O   HOH I 750      82.632  29.387  54.649  1.00 21.70           O
ANISOU39810  O   HOH I 750     2273   2644   3327   -171   -296    149      O
ATOM  39849  O   HOH I 763      76.456  11.744  48.843  1.00 29.61           O
ANISOU39849  O   HOH I 763     3768   3512   3968   -302   -130   -155      O
ATOM  39864  O   HOH I 768      75.026  25.830  39.829  1.00 31.65           O
ANISOU39864  O   HOH I 768     4316   3653   4056    -94   -213    -49      O
ATOM  39897  O   HOH I 779      76.219  13.476  52.729  1.00 25.96           O
ANISOU39897  O   HOH I 779     2493   3855   3514    235    390   -200      O
ATOM  40059  O   HOH I 833      80.573  21.969  45.066  1.00 24.01           O
ANISOU40059  O   HOH I 833     3003   3043   3073    235    142    -17      O
ATOM  40074  O   HOH I 838      87.060  27.226  37.189  1.00 33.33           O
ANISOU40074  O   HOH I 838     4406   4189   4067    152    -96   -109      O
ATOM  40128  O   HOH I 856      77.486  12.237  46.550  1.00 34.07           O
ANISOU40128  O   HOH I 856     3948   4240   4755      3    103   -123      O
ATOM  40353  O   HOH I 931      67.083  29.743  35.307  1.00 38.75           O
ANISOU40353  O   HOH I 931     4740   5143   4841    -97   -162    -50      O
ATOM  40356  O   HOH I 932      79.944  21.840  60.235  1.00 29.91           O
ANISOU40356  O   HOH I 932     3908   3445   4011     86     18    114      O
ATOM  40434  O   HOH I 958      88.819  33.122  46.420  1.00 27.10           O
ANISOU40434  O   HOH I 958     3228   3067   3998    197    737    176      O
ATOM  40446  O   HOH I 962      61.700  24.339  37.540  1.00 29.91           O
ANISOU40446  O   HOH I 962     3676   3915   3774   -405   -201   -200      O
ATOM  40452  O   HOH I 964      79.036  10.825  50.418  1.00 32.30           O
ANISOU40452  O   HOH I 964     4456   3475   4341    283   -120     26      O
ATOM  40476  O   HOH I 972      66.603  18.545  39.877  0.00 28.19           O
ANISOU40476  O   HOH I 972     3635   3912   3165    287    234     75      O
ATOM  40635  O   HOH I1025     75.973  11.924  56.867  1.00 28.27           O
ANISOU40635  O   HOH I1025     3373   3496   3869    379    234    170      O
ATOM  40653  O   HOH I1031     86.010  13.779  51.750  1.00 37.18           O
ANISOU40653  O   HOH I1031     4682   4608   4833     59    109     65      O
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ATOM	40767	O	HOH	I1069	79.787	40.960	58.104	1.00	36.42			O
ANISOU	40767	O	HOH	I1069	4339	4769	4730	334	86	13		O
ATOM	40806	O	HOH	I1082	84.999	17.603	52.422	1.00	27.50			O
ANISOU	40806	O	HOH	I1082	3243	3267	3937	-72	-17	139		O
ATOM	40833	O	HOH	I1091	84.459	27.235	60.441	1.00	30.28			O
ANISOU	40833	O	HOH	I1091	3698	3634	4172	87	-74	289		O
ATOM	41034	O	HOH	I1158	69.604	16.212	47.222	1.00	32.38			O
ANISOU	41034	O	HOH	I1158	4183	4264	3856	316	-32	-7		O
ATOM	41214	O	HOH	I1218	70.544	29.378	40.838	1.00	34.08			O
ANISOU	41214	O	HOH	I1218	4076	4501	4370	-74	71	-38		O
ATOM	41307	O	HOH	I1249	77.720	15.022	54.382	1.00	25.01			O
ANISOU	41307	O	HOH	I1249	3839	2205	3455	0	315	193		O
ATOM	41376	O	HOH	I1272	92.164	29.566	60.811	1.00	41.16			O
ANISOU	41376	O	HOH	I1272	5062	5054	5520	4	187	-40		O
ATOM	41391	O	HOH	I1277	78.225	35.244	37.422	1.00	45.50			O
ANISOU	41391	O	HOH	I1277	5680	5687	5920	-30	96	96		O
ATOM	41412	O	HOH	I1284	62.209	24.973	34.838	1.00	49.83			O
ANISOU	41412	O	HOH	I1284	6142	6402	6390	9	3	-49		O
ATOM	41415	O	HOH	I1285	78.559	31.939	37.407	1.00	35.91			O
ANISOU	41415	O	HOH	I1285	4282	4680	4680	-172	12	65		O
ATOM	41481	O	HOH	I1307	83.630	23.857	43.928	1.00	39.19			O
ANISOU	41481	O	HOH	I1307	4814	5426	4650	149	60	100		O
ATOM	41529	O	HOH	I1323	99.439	23.637	54.905	1.00	25.19			O
ANISOU	41529	O	HOH	I1323	3392	3000	3180	49	-4	173		O
ATOM	41613	O	HOH	I1351	78.713	22.034	39.915	1.00	49.57			O
ANISOU	41613	O	HOH	I1351	6252	6307	6272	-17	77	-4		O
ATOM	41718	O	HOH	I1386	78.105	20.078	42.022	1.00	38.92			O
ANISOU	41718	O	HOH	I1386	5107	4908	4771	-99	62	123		O
ATOM	41736	O	HOH	I1392	83.573	16.260	46.747	1.00	39.58			O
ANISOU	41736	O	HOH	I1392	5199	4912	4926	92	-150	10		O
ATOM	41766	O	HOH	I1402	65.274	25.273	36.276	1.00	30.66			O
ANISOU	41766	O	HOH	I1402	3979	4087	3582	-499	117	-181		O
ATOM	41775	O	HOH	I1405	63.905	25.981	33.612	1.00	60.85			O
ANISOU	41775	O	HOH	I1405	7711	7766	7640	0	81	-2		O
ATOM	41865	O	HOH	I1435	72.974	15.861	47.445	1.00	29.87			O
ANISOU	41865	O	HOH	I1435	4082	3226	4040	82	-147	-87		O
ATOM	41889	O	HOH	I1443	88.700	26.970	34.611	1.00	46.25			O
ANISOU	41889	O	HOH	I1443	5763	5989	5822	-21	-12	13		O
ATOM	42012	O	HOH	I1484	91.890	14.843	45.880	1.00	30.33			O
ANISOU	42012	O	HOH	I1484	3968	3237	4318	-203	100	-123		O
ATOM	42078	O	HOH	I1506	64.224	14.605	43.908	1.00	39.80			O
ANISOU	42078	O	HOH	I1506	4983	5352	4785	-35	61	-96		O
ATOM	42186	O	HOH	I1542	85.452	24.536	42.808	1.00	35.53			O
ANISOU	42186	O	HOH	I1542	4291	4665	4542	-383	-1	-16		O
ATOM	42393	O	HOH	I1611	66.209	22.296	39.786	1.00	36.50			O
ANISOU	42393	O	HOH	I1611	4914	4434	4519	-37	109	-50		O
ATOM	42396	O	HOH	I1612	67.389	15.483	40.662	1.00	51.12			O
ANISOU	42396	O	HOH	I1612	6740	6398	6284	-84	85	0		O
ATOM	42405	O	HOH	I1615	92.896	23.214	35.963	1.00	46.09			O
ANISOU	42405	O	HOH	I1615	6086	5617	5808	-30	-73	-223		O
ATOM	42435	O	HOH	I1625	86.422	25.216	40.369	1.00	46.61			O
ANISOU	42435	O	HOH	I1625	5836	5970	5900	-150	82	34		O
ATOM	42516	O	HOH	I1652	68.375	14.168	47.274	1.00	27.12			O
ANISOU	42516	O	HOH	I1652	3886	3475	2942	382	42	366		O
ATOM	42783	O	HOH	I1741	80.971	19.555	45.297	1.00	60.76			O
ANISOU	42783	O	HOH	I1741	7717	7577	7790	5	-10	12		O
ATOM	42831	O	HOH	I1757	87.332	14.976	47.405	1.00	47.04			O
ANISOU	42831	O	HOH	I1757	5977	5977	5919	-43	-126	74		O
ATOM	42846	O	HOH	I1762	76.590	10.990	52.768	1.00	44.72			O
ANISOU	42846	O	HOH	I1762	5801	5563	5625	-63	93	-23		O
ATOM	42882	O	HOH	I1774	93.494	20.613	37.093	1.00	44.76			O

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ANISOU42882  O   HOH I1774     5535   5819   5652   -165     94     23        O
ATOM  42969  O   HOH I1803      79.512  31.284  34.819  1.00 43.33           O
ANISOU42969  O   HOH I1803     5406   5557   5499     -7   -283     26        O
ATOM  43029  O   HOH I1823      74.883  17.439  45.078  1.00 49.34           O
ANISOU43029  O   HOH I1823     6136   6423   6186     82    -97     18        O
ATOM  43158  O   HOH I1866      82.139  27.856  33.595  1.00 29.87           O
ANISOU43158  O   HOH I1866     4055   3717   3576   -333     87   -286        O
ATOM  43293  O   HOH I1911      79.150  26.600  33.773  1.00 41.61           O
ANISOU43293  O   HOH I1911     5570   5292   4948   -109   -156    -29        O
ATOM  43305  O   HOH I1915      78.277  19.001  44.635  1.00 41.86           O
ANISOU43305  O   HOH I1915     5361   5267   5276    154     87   -104        O
ATOM  43422  O   HOH I1954      80.021  12.895  46.345  1.00 53.52           O
ANISOU43422  O   HOH I1954     6638   7049   6646    -63    128     68        O
ATOM  43554  O   HOH I1998      81.100  16.776  46.759  1.00 43.92           O
ANISOU43554  O   HOH I1998     5602   5605   5478    -61    138   -165        O
ATOM  43617  O   HOH I2019      91.203  22.559  37.690  1.00 48.97           O
ANISOU43617  O   HOH I2019     6251   6031   6322     31     64    -62        O
ATOM  43755  O   HOH I2065      66.142  18.386  34.319  1.00 48.98           O
ANISOU43755  O   HOH I2065     6185   6442   5982      6    -32    -23        O
ATOM  43836  O   HOH I2092      80.735  22.143  42.477  1.00 37.19           O
ANISOU43836  O   HOH I2092     4728   4763   4636    133      5   -182        O
ATOM  43875  O   HOH I2105      83.915  26.626  32.072  1.00 45.21           O
ANISOU43875  O   HOH I2105     5953   5465   5757   -117    165    -35        O
ATOM  43905  O   HOH I2115      83.540  25.970  35.651  1.00 46.05           O
ANISOU43905  O   HOH I2115     5968   5643   5884     50    -42   -133        O
ATOM  43956  O   HOH I2132      82.824  34.749  33.460  1.00 34.25           O
ANISOU43956  O   HOH I2132     4486   4435   4092     37   -105   -134        O
ATOM  43965  O   HOH I2135      68.875  13.908  44.337  1.00 53.45           O
ANISOU43965  O   HOH I2135     6754   6694   6859   -116    124   -141        O
ATOM  43983  O   HOH I2141      84.555  23.000  39.511  1.00 35.28           O
ANISOU43983  O   HOH I2141     3621   4916   4868   -159    195    156        O
ATOM  44025  O   HOH I2155      68.212  11.904  44.669  1.00 68.29           O
ANISOU44025  O   HOH I2155     8775   8627   8544    -34     36     -9        O
ATOM  44289  O   HOH I2243      70.303  18.163  43.625  1.00 44.02           O
ANISOU44289  O   HOH I2243     5768   5477   5481     32      3    -26        O
ATOM  44340  O   HOH I2260      77.299  11.249  43.900  1.00 62.73           O
ANISOU44340  O   HOH I2260     7898   8068   7869    -24     -7     14        O
ATOM  44352  O   HOH I2264      91.547  12.409  46.194  1.00 47.48           O
ANISOU44352  O   HOH I2264     6013   5720   6304    -85    -85     47        O
ATOM  44421  O   HOH I2287      66.076  22.939  34.318  1.00 47.34           O
ANISOU44421  O   HOH I2287     5956   6051   5978   -133    -17     -1        O
ATOM  44658  O   HOH I2366      92.333  40.065  50.189  1.00 40.05           O
ANISOU44658  O   HOH I2366     5206   4957   5051    -81    144   -124        O
ATOM  44781  O   HOH I2407      84.696  24.577  61.147  1.00 46.09           O
ANISOU44781  O   HOH I2407     5865   5622   6025     -2    -67    154        O
ATOM  45048  O   HOH I2496      71.587  15.143  43.827  1.00 42.91           O
ANISOU45048  O   HOH I2496     5416   5554   5332      9   -293    -85        O
ATOM  45087  O   HOH I2509      68.877  34.391  33.745  1.00 48.68           O
ANISOU45087  O   HOH I2509     6052   6308   6134    -79    -37    -51        O
ATOM  45126  O   HOH I2522      64.649  32.366  36.686  1.00 52.30           O
ANISOU45126  O   HOH I2522     6567   6707   6597    -33    -76    -45        O
ATOM  45300  O   HOH I2580      86.072  21.234  62.272  1.00 40.57           O
ANISOU45300  O   HOH I2580     4898   5267   5250     88     43     31        O
ATOM  45753  O   HOH I2731      64.365  21.736  33.031  1.00 40.46           O
ANISOU45753  O   HOH I2731     4897   5185   5289    -12    -20     17        O
ATOM  46146  O   HOH I2862      68.349  14.962  32.720  1.00 41.81           O
ANISOU46146  O   HOH I2862     5292   5631   4962    -79     11   -110        O
ATOM  46188  O   HOH I2876      85.649  15.223  40.779  1.00 62.78           O
ANISOU46188  O   HOH I2876     7864   7929   8058      4    -15    -74        O
ATOM  46293  O   HOH I2911      92.232  29.400  34.253  1.00 41.62           O
ANISOU46293  O   HOH I2911     4973   5606   5234   -145     33    -47        O
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ATOM  46464  O   HOH I2968      85.429  20.036  51.002  1.00 25.74           O
ANISOU46464  O   HOH I2968    3335   2889   3554    -32    -69   -133        O
END
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Annex 1 Cont'd : 70

ACTIVE SITES

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REMARK Created by MOLEMAN2 V. 990504/2.3 at Thu Jul 13 16:59:24 2000 for wulf
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3   Maximum likelihood refinement was used
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.7
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 73.
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.0
REMARK   3   COMPLETENESS FOR RANGE        (%) : 82.7
REMARK   3   NUMBER OF REFLECTIONS             :. 230146
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE      (WORKING + TEST SET) : 0.16587
REMARK   3   R VALUE            (WORKING SET) : 0.16312
REMARK   3   FREE R VALUE                      : 0.21818
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :5.0
REMARK   3   FREE R VALUE TEST SET COUNT      :12192
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   All atoms                 :   46517
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 14.387
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    0.46
REMARK   3    B22 (A**2) :   -0.19
REMARK   3    B33 (A**2) :   -0.27
REMARK   3    B12 (A**2) :    0.03
REMARK   3    B13 (A**2) :   -0.02
REMARK   3    B23 (A**2) :   -0.25
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                (A):
REMARK   3  NULL
REMARK   3   ESU BASED ON FREE R VALUE                           (A):
REMARK   3   0.18277
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                     (A):
REMARK   3   0.12940
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):
REMARK   3   8.01924
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   DISTANCE RESTRAINTS.                      RMS    SIGMA
REMARK   3    BOND LENGTH                    (A)  : 0.021 ; 0.021
REMARK   3    BOND ANGLE                (DEGREES) : 2.076 ; 2.015
REMARK   3    Torsion angles, period 1  (DEGREES) : 5.103 ; 3.000
REMARK   3    Torsion angles, period 3  (DEGREES) :16.457 ;15.000
REMARK   3    CHIRAL-CENTER RESTRAINTS     (A**3) : 0.126 ; 0.200
REMARK   3    PLANE RESTRAINT                (A)  : 0.009 ; 0.020
REMARK   3    VDW repulsions                 (A)  : 0.232 ; 0.300
REMARK   3    Potential hbonds               (A)  : 0.217 ; 0.500
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS    SIGMA
REMARK   3   MAIN-CHAIN BOND                (A**2) : 1.443 ; 1.500
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REMARK   3   MAIN-CHAIN ANGLE                (A**2) : 2.158 ; 2.000
REMARK   3   SIDE-CHAIN BOND                 (A**2) : 3.125 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE                (A**2) : 4.584 ; 4.500
REMARK   3
REMARK   3 ANISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS     SIGMA
REMARK   3   Rigid-bond restraints           (A**2) : 1.894 ; 2.000
REMARK   3   Sphericity; free atoms          (A**2) : 4.664 ; 2.000
REMARK   3   Sphericity; bondec atoms        (A**2) : 2.553 ; 2.000
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS.
REMARK   3
REMARK   3  TLS details
REMARK   3  Number of tls groups                  :   8
REMARK   3
REMARK   3  Number of pieces in the TLS group    1:    1
REMARK   3  From A   1 to A 292
REMARK   3  Origin for the group                  :   1
REMARK   3   69.4830  59.4220  78.9970
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0325  0.0433  0.0247 -0.0039 -0.0136 -0.0012
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6102  0.6435  0.4229 -0.1271  0.0884 -0.0867
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3   0.0248 -0.0135 -0.0505  0.0232  0.0615 -0.0461  0.0207 -0.0758
REMARK   3
REMARK   3  Number of pieces in the TLS group    2:    1
REMARK   3  From B   1 to B 293
REMARK   3  Origin for the group                  :   2
REMARK   3   61.2650  33.4890  54.1360
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0294  0.0510  0.0183  0.0014  0.0082 -0.0045
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6794  0.6303  0.4419  0.1224 -0.1618 -0.1218
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0046 -0.0119  0.0109  0.0234  0.0528  0.0423 -0.0173 -0.0642
REMARK   3
REMARK   3  Number of pieces in the TLS group    3:    1
REMARK   3  From C   1 to C 292
REMARK   3  Origin for the group                  :   3
REMARK   3  100.4020  45.2900  79.2890
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0309  0.0357  0.0395  0.0126  0.0217  0.0172
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.5756  0.7497  0.6477 -0.1840  0.0581 -0.3103
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0999 -0.0112  0.0060  0.0283 -0.1071 -0.0800  0.0406  0.0887
REMARK   3
REMARK   3  Number of pieces in the TLS group    4:    1
REMARK   3  From D   1 to D 292
REMARK   3  Origin for the group                  :   4
REMARK   3   93.1810  38.1690  43.3930
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3   0.0110  0.0453  0.0536  0.0109  0.0225  0.0295
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3   0.6426  0.7184  0.8911  0.0882 -0.0950 -0.4089
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.1237 -0.0615  0.0018 -0.0411 -0.1339 -0.0574  0.0193  0.1369
REMARK   3
REMARK   3  Number of pieces in the TLS group    5:    1
REMARK   3  From E   1 to E 292
REMARK   3  Origin for the group                  :   5
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REMARK   3    42.8770    8.9030  19.5730
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0309   0.0452   0.0352   0.0089 -0.0125 -0.0200
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.6312   0.7631   0.9845   0.0814   0.0288   0.4970
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.1195 -0.0434 -0.0468   0.0342   0.1311 -0.0463 -0.0408 -0.1559
REMARK   3
REMARK   3  Number of pieces in the TLS group     6:     1
REMARK   3  From F    1 to F 293
REMARK   3  Origin for the group                  :    6
REMARK   3    38.0920   17.7800 -16.3490
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0208   0.0425   0.0417   0.0034   0.0045 -0.0015
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.8800   0.3582   0.6933   0.1180   0.1354   0.1904
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0810   0.0464 -0.0329   0.0291   0.0416   0.0160 -0.0440 -0.0740
REMARK   3
REMARK   3  Number of pieces in the TLS group     7:     1
REMARK   3  From G    1 to G 292
REMARK   3  Origin for the group                  :    7
REMARK   3    71.8950   21.8640 -15.9250
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0234   0.0522   0.0272 -0.0024 -0.0109   0.0094
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.5696   0.5742   0.4250   0.0699 -0.0286 -0.0019
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0333   0.0146   0.0152 -0.0110 -0.0283   0.0204 -0.0007   0.0589
REMARK   3
REMARK   3  Number of pieces in the TLS group     8:     1
REMARK   3  From H    1 to H 292
REMARK   3  Origin for the group                  :    8
REMARK   3    71.9070   -5.2410    8.8240
REMARK   3  T tensor (T11, T22, T33, T12, T13, T23)
REMARK   3    0.0445   0.0386   0.0064   0.0038   0.0132   0.0109
REMARK   3  L tensor (L11, L22, L33, L12, L13, L23)
REMARK   3    0.4837   0.7743   0.6523 -0.1036 -0.1161   0.0699
REMARK   3  S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK   3  -0.0109 -0.0288 -0.0166   0.0049 -0.0575 -0.0486   0.0096   0.0981
REMARK   3
REMARK   3  Hydrogens have been added in the riding positions
REMARK   3
REMARK   3
REMARK   3              Scaling details
REMARK   3  Babinet"s principle for scaling has been used
REMARK   3  Bulk solvent correction based on constant value has been used
REMARK   3  Parameters for mask calculation
REMARK   3   VDW prob radii   =   1.40
REMARK   3   ION prob radii   =   0.80
REMARK   3   Shrinkage radii  =   0.80
REMARK   3
HEADER    ----                                        XX-XXX-XX    xxxx
COMPND    ---
CISPEP   1 HIS A   16     PRO A   17                      0.00
CISPEP   2 HIS B   17     PRO B   18                      0.00
CISPEP   3 HIS C   16     PRO C   17                      0.00
CISPEP   4 HIS D   16     PRO D   17                      0.00
CISPEP   5 HIS E   16     PRO E   17                      0.00
CISPEP   6 HIS G   16     PRO G   17                      0.00
CISPEP   7 HIS H   16     PRO H   17                      0.00
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CISPEP   8 HIS F   17    PRO F   18                    0.00
CRYST1   71.575   73.410  134.290  89.94  80.61  80.93 P 1           1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.013971 -0.002230 -0.002368        0.00000
SCALE2      0.000000  0.013795  0.000349        0.00000
SCALE3      0.000000  0.000000  0.007550        0.00000
ATOM    328  CD1 ILE A  22      59.967  47.366  65.615  1.00 33.85           C
ANISOU  328  CD1 ILE A  22    4267   4278   4314     26     53    -50       C
ATOM    432  CG  PRO A  28      66.308  45.162  69.043  1.00 13.58           C
ANISOU  432  CG  PRO A  28    1807   1645   1708     59    -94    -91       C
ATOM   4272  N   LYS A 276      63.617  31.206  81.166  1.00 20.93           N
ANISOU 4272  N   LYS A 276    2678   2673   2601    -66     43    -61       N
ATOM   4274  CA  LYS A 276      63.911  30.276  80.088  1.00 22.01           C
ANISOU 4274  CA  LYS A 276    2776   2842   2744    -36     48    -29       C
ATOM   4276  CB  LYS A 276      62.666  29.928  79.262  1.00 22.43           C
ANISOU 4276  CB  LYS A 276    2800   2903   2817    -15    -31    -11       C
ATOM   4279  CG  LYS A 276      61.548  29.173  80.028  1.00 24.80           C
ANISOU 4279  CG  LYS A 276    3078   3271   3071    -51    104     -9       C
ATOM   4282  CD  LYS A 276      61.850  27.689  80.289  1.00 28.12           C
ANISOU 4282  CD  LYS A 276    3580   3521   3582    -14     38     85       C
ATOM   4285  CE  LYS A 276      61.479  26.778  79.084  1.00 30.97           C
ANISOU 4285  CE  LYS A 276    4025   3975   3765    -22     -7    -28       C
ATOM   4288  NZ  LYS A 276      61.473  25.294  79.348  1.00 33.41           N
ANISOU 4288  NZ  LYS A 276    4357   4145   4192     -1      0     31       N
ATOM   4292  C   LYS A 276      64.962  30.874  79.183  1.00 21.47           C
ANISOU 4292  C   LYS A 276    2695   2761   2698    -38     27    -49       C
ATOM   4293  O   LYS A 276      65.346  30.254  78.213  1.00 21.93           O
ANISOU 4293  O   LYS A 276    2808   2846   2675   -109    -37   -263       O
ATOM   4294  N   ASN A 277      65.439  32.067  79.497  1.00 20.65           N
ANISOU 4294  N   ASN A 277    2652   2640   2551      6    -13    -71       N
ATOM   4296  CA  ASN A 277      66.438  32.690  78.652  1.00 19.73           C
ANISOU 4296  CA  ASN A 277    2515   2478   2503    -15    -15    -54       C
ATOM   4298  CB  ASN A 277      65.754  33.728  77.777  1.00 20.79           C
ANISOU 4298  CB  ASN A 277    2641   2661   2597      4    -33    -11       C
ATOM   4301  CG  ASN A 277      64.999  34.796  78.617  1.00 22.82           C
ANISOU 4301  CG  ASN A 277    2899   2803   2968     -5    -62   -172       C
ATOM   4302  OD1 ASN A 277      65.656  35.665  79.160  1.00 20.73           O
ANISOU 4302  OD1 ASN A 277    2630   2112   3134   -213    -58    282       O
ATOM   4303  ND2 ASN A 277      63.604  34.677  78.777  1.00 23.06           N
ANISOU 4303  ND2 ASN A 277    2877   3050   2833   -178     34    -47       N
ATOM   4306  C   ASN A 277      67.629  33.274  79.432  1.00 19.02           C
ANISOU 4306  C   ASN A 277    2493   2406   2327     57      7    -31       C
ATOM   4308  N   GLY A 278      68.634  33.764  78.693  1.00 16.96           N
ANISOU 4308  N   GLY A 278    2237   2114   2091    -42    -46    -54       N
ATOM   4654  CA  GLY B   5      53.052  32.510  49.620  1.00  8.62           C
ANISOU 4654  CA  GLY B   5    1034   1119   1121    131     38     18       C
ATOM   4657  C   GLY B   5      52.521  32.740  51.044  1.00  8.23           C
ANISOU 4657  C   GLY B   5    1027   1023   1078     21    -26   -110       C
ATOM   4658  O   GLY B   5      51.452  33.330  51.223  1.00  7.96           O
ANISOU 4658  O   GLY B   5    861   1053   1109     99    -52   -212       O
ATOM   4659  N   ILE B   6      53.253  32.209  52.017  1.00  7.06           N
ANISOU 4659  N   ILE B   6    713    943   1026     57     58    -14       N
ATOM   4661  CA  ILE B   6      53.005  32.398  53.422  1.00  7.81           C
ANISOU 4661  CA  ILE B   6    893   1031   1042     62    -58    -29       C
ATOM   4663  CB  ILE B   6      52.441  31.143  54.056  1.00  7.78           C
ANISOU 4663  CB  ILE B   6    920   1034   1000    102   -106     -1       C
ATOM   4665  CG1 ILE B   6      51.270  30.624  53.275  1.00 10.95           C
ANISOU 4665  CG1 ILE B   6   1124   1370   1665    -16    -74    -78       C
ATOM   4668  CD1 ILE B   6      50.634  29.447  53.966  1.00 11.37           C
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ANISOU	4668	CD1	ILE	B	6	1342	1616	1360	-189	-124	98		C
ATOM	4672	CG2	ILE	B	6	52.085	31.412	55.516	1.00	8.38			C
ANISOU	4672	CG2	ILE	B	6	966	1112	1106	36	-72	121		C
ATOM	4676	C	ILE	B	6	54.268	32.714	54.166	1.00	7.81			C
ANISOU	4676	C	ILE	B	6	872	1070	1023	17	39	66		C
ATOM	4677	O	ILE	B	6	55.322	32.027	53.970	1.00	9.13			O
ANISOU	4677	O	ILE	B	6	877	1163	1430	180	-200	39		O
ATOM	4678	N	ILE	B	7	54.186	33.767	54.973	1.00	8.62			N
ANISOU	4678	N	ILE	B	7	867	1194	1213	149	-99	30		N
ATOM	4680	CA	ILE	B	7	55.273	34.105	55.910	1.00	9.24			C
ANISOU	4680	CA	ILE	B	7	1136	1235	1137	41	-23	14		C
ATOM	4682	CB	ILE	B	7	55.694	35.537	55.868	1.00	10.30			C
ANISOU	4682	CB	ILE	B	7	1301	1421	1190	-18	-22	-15		C
ATOM	4684	CG1	ILE	B	7	56.111	35.974	54.453	1.00	10.33			C
ANISOU	4684	CG1	ILE	B	7	1317	1288	1319	93	210	102		C
ATOM	4687	CD1	ILE	B	7	56.320	37.425	54.375	1.00	10.11			C
ANISOU	4687	CD1	ILE	B	7	1084	1503	1253	-195	311	117		C
ATOM	4691	CG2	ILE	B	7	56.887	35.764	56.869	1.00	9.63			C
ANISOU	4691	CG2	ILE	B	7	1070	1233	1356	80	-151	-68		C
ATOM	4695	C	ILE	B	7	54.804	33.759	57.296	1.00	8.87			C
ANISOU	4695	C	ILE	B	7	1024	1198	1147	20	45	-4		C
ATOM	4696	O	ILE	B	7	53.848	34.341	57.766	1.00	7.45			O
ANISOU	4696	O	ILE	B	7	488	1146	1196	-11	50	146		O
ATOM	4697	N	LEU	B	8	55.547	32.872	57.988	1.00	8.33			N
ANISOU	4697	N	LEU	B	8	911	1085	1168	68	67	36		N
ATOM	4699	CA	LEU	B	8	55.220	32.551	59.377	1.00	8.71			C
ANISOU	4699	CA	LEU	B	8	886	1279	1145	1	15	17		C
ATOM	4701	CB	LEU	B	8	55.444	31.085	59.673	1.00	8.42			C
ANISOU	4701	CB	LEU	B	8	848	1164	1186	83	12	-61		C
ATOM	4704	CG	LEU	B	8	54.937	30.427	60.947	1.00	13.63			C
ANISOU	4704	CG	LEU	B	8	1659	1822	1697	42	33	-9		C
ATOM	4706	CD1	LEU	B	8	53.455	30.654	61.157	1.00	13.18			C
ANISOU	4706	CD1	LEU	B	8	1440	1872	1693	17	67	134		C
ATOM	4710	CD2	LEU	B	8	55.189	28.950	61.003	1.00	14.77			C
ANISOU	4710	CD2	LEU	B	8	1701	1898	2011	197	-83	33		C
ATOM	4714	C	LEU	B	8	56.066	33.473	60.246	1.00	8.77			C
ANISOU	4714	C	LEU	B	8	1016	1241	1073	9	19	117		C
ATOM	4715	O	LEU	B	8	57.309	33.329	60.288	1.00	8.90			O
ANISOU	4715	O	LEU	B	8	772	1585	1022	-62	-80	134		O
ATOM	4716	N	ALA	B	9	55.418	34.470	60.831	1.00	9.86			N
ANISOU	4716	N	ALA	B	9	989	1477	1279	-44	84	24		N
ATOM	4718	CA	ALA	B	9	56.095	35.542	61.548	1.00	10.37			C
ANISOU	4718	CA	ALA	B	9	1209	1347	1384	47	12	-2		C
ATOM	4720	CB	ALA	B	9	55.998	36.760	60.777	1.00	11.75			C
ANISOU	4720	CB	ALA	B	9	1343	1553	1569	51	-52	-55		C
ATOM	4724	C	ALA	B	9	55.607	35.757	62.965	1.00	11.00			C
ANISOU	4724	C	ALA	B	9	1263	1421	1494	43	-9	-34		C
ATOM	4725	O	ALA	B	9	55.473	36.905	63.428	1.00	11.38			O
ANISOU	4725	O	ALA	B	9	1194	1494	1636	-105	-33	-67		O
ATOM	4726	N	GLY	B	10	55.253	34.650	63.604	1.00	11.58			N
ANISOU	4726	N	GLY	B	10	1334	1459	1606	-26	-27	-33		N
ATOM	4728	CA	GLY	B	10	54.806	34.643	64.955	1.00	12.14			C
ANISOU	4728	CA	GLY	B	10	1404	1614	1594	-11	-36	-9		C
ATOM	4731	C	GLY	B	10	55.867	34.159	65.918	1.00	13.80			C
ANISOU	4731	C	GLY	B	10	1615	1866	1759	-55	-98	9		C
ATOM	4732	O	GLY	B	10	57.042	34.470	65.782	1.00	10.83			O
ANISOU	4732	O	GLY	B	10	1024	1785	1305	91	-348	-50		O
ATOM	4733	N	GLY	B	11	55.441	33.393	66.902	1.00	15.86			N
ANISOU	4733	N	GLY	B	11	1891	2141	1993	-145	-64	98		N
ATOM	4735	CA	GLY	B	11	56.356	32.896	67.932	1.00	18.72			C
ANISOU	4735	CA	GLY	B	11	2268	2394	2451	-69	-72	89		C

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ATOM   4738  C   GLY B  11      56.583  33.905  69.053  1.00 21.22           C
ANISOU 4738  C   GLY B  11    2691   2766   2602      5    -29    -24        C
ATOM   4739  O   GLY B  11      56.307  35.125  68.902  1.00 21.22           O
ANISOU 4739  O   GLY B  11    2619   2925   2517     37   -175    -28        O
ATOM   4740  N   SER B  12      57.164  33.401  70.145  1.00 24.10           N
ANISOU 4740  N   SER B  12    3060   3108   2988     66    -56     31        N
ATOM   4742  CA  SER B  12      57.398  34.142  71.396  1.00 25.99           C
ANISOU 4742  CA  SER B  12    3317   3290   3268     53    -70      7        C
ATOM   4744  CB  SER B  12      57.390  33.084  72.522  1.00 27.20           C
ANISOU 4744  CB  SER B  12    3513   3488   3331     34     34     26        C
ATOM   4747  OG  SER B  12      58.313  32.017  72.217  1.00 31.02           O
ANISOU 4747  OG  SER B  12    3951   3661   4174    130   -145    -14        O
ATOM   4749  C   SER B  12      58.711  34.979  71.435  1.00 26.05           C
ANISOU 4749  C   SER B  12    3296   3334   3265     74    -62    -16        C
ATOM   4750  O   SER B  12      58.847  35.965  72.200  1.00 27.75           O
ANISOU 4750  O   SER B  12    3451   3458   3631    109   -142     53        O
ATOM   4751  N   GLY B  13      59.695  34.585  70.640  1.00 25.18           N
ANISOU 4751  N   GLY B  13    3171   3282   3114     31   -100     18        N
ATOM   4753  CA  GLY B  13      60.978  35.257  70.614  1.00 24.90           C
ANISOU 4753  CA  GLY B  13    3228   3139   3092    -17    -53      4        C
ATOM   4756  C   GLY B  13      61.702  35.190  71.959  1.00 24.18           C
ANISOU 4756  C   GLY B  13    3041   3069   3077     14    -79     36        C
ATOM   4757  O   GLY B  13      62.504  36.091  72.293  1.00 24.09           O
ANISOU 4757  O   GLY B  13    3096   2846   3208    -12    -13     99        O
ATOM   4758  N   THR B  14      61.418  34.155  72.747  1.00 23.43           N
ANISOU 4758  N   THR B  14    2934   2945   3024    -75    -73    -14        N
ATOM   4760  CA  THR B  14      62.039  33.999  74.095  1.00 23.26           C
ANISOU 4760  CA  THR B  14    2917   2923   2997     -2    -47     10        C
ATOM   4762  CB  THR B  14      61.656  32.636  74.640  1.00 23.77           C
ANISOU 4762  CB  THR B  14    2909   3078   3042    -31     24     30        C
ATOM   4764  OG1 THR B  14      60.232  32.596  74.876  1.00 25.47           O
ANISOU 4764  OG1 THR B  14    2930   3108   3640     71    -29     49        O
ATOM   4766  CG2 THR B  14      62.232  32.400  75.994  1.00 24.62           C
ANISOU 4766  CG2 THR B  14    3048   3159   3147    -45      7     46        C
ATOM   4770  C   THR B  14      63.573  34.206  74.114  1.00 23.18           C
ANISOU 4770  C   THR B  14    2944   2938   2924    -11     -8     -4        C
ATOM   4771  O   THR B  14      64.134  34.980  74.942  1.00 22.98           O
ANISOU 4771  O   THR B  14    2877   2886   2968    -24    -38    -97        O
ATOM   4772  N   ARG B  15      64.293  33.558  73.220  1.00 22.84           N
ANISOU 4772  N   ARG B  15    2926   2824   2926      4    -36    -58        N
ATOM   4774  CA  ARG B  15      65.765  33.741  73.237  1.00 23.13           C
ANISOU 4774  CA  ARG B  15    2934   2881   2971    -18    -23    -18        C
ATOM   4776  CB  ARG B  15      66.438  32.910  72.162  1.00 24.19           C
ANISOU 4776  CB  ARG B  15    3004   3059   3125      3    -20    -71        C
ATOM   4779  CG  ARG B  15      66.233  31.423  72.405  1.00 26.14           C
ANISOU 4779  CG  ARG B  15    3334   3177   3418     -5     -8     66        C
ATOM   4782  CD  ARG B  15      66.636  30.526  71.228  1.00 30.66           C
ANISOU 4782  CD  ARG B  15    3916   3876   3855     71     80    -99        C
ATOM   4785  NE  ARG B  15      65.682  30.594  70.127  1.00 33.05           N
ANISOU 4785  NE  ARG B  15    4150   4267   4139     36     23    -43        N
ATOM   4787  CZ  ARG B  15      65.992  30.490  68.841  1.00 34.85           C
ANISOU 4787  CZ  ARG B  15    4461   4409   4372    -28     12      3        C
ATOM   4788  NH1 ARG B  15      67.267  30.299  68.467  1.00 36.37           N
ANISOU 4788  NH1 ARG B  15    4506   4533   4777    -35    108     25        N
ATOM   4791  NH2 ARG B  15      65.028  30.565  67.928  1.00 33.50           N
ANISOU 4791  NH2 ARG B  15    4310   4098   4318    -57    -27     21        N
ATOM   4794  C   ARG B  15      66.232  35.222  73.153  1.00 22.53           C
ANISOU 4794  C   ARG B  15    2842   2821   2895      1    -14    -23        C
ATOM   4795  O   ARG B  15      67.323  35.575  73.649  1.00 21.79           O
ANISOU 4795  O   ARG B  15    2737   2767   2773    -37     52    -36        O
ATOM   4796  N   LEU B  16      65.387  36.088  72.591  1.00 21.89           N
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ANISOU 4796  N   LEU B  16     2815   2704   2799    -71    -78    -12       N
ATOM   4798  CA  LEU B  16      65.751  37.502  72.466  1.00 21.56           C
ANISOU 4798  CA  LEU B  16     2763   2676   2750     13    -63     37       C
ATOM   4800  CB  LEU B  16      65.338  38.016  71.098  1.00 20.99           C
ANISOU 4800  CB  LEU B  16     2564   2721   2688     21    -56     13       C
ATOM   4803  CG  LEU B  16      66.028  37.289  69.966  1.00 22.08           C
ANISOU 4803  CG  LEU B  16     2675   2893   2821     10    -39     -8       C
ATOM   4805  CD1 LEU B  16      65.480  37.772  68.657  1.00 23.18           C
ANISOU 4805  CD1 LEU B  16     2789   3105   2913    102      7     13       C
ATOM   4809  CD2 LEU B  16      67.595  37.513  70.012  1.00 23.46           C
ANISOU 4809  CD2 LEU B  16     2847   3058   3009     -3    -22    -99       C
ATOM   4813  C   LEU B  16      65.280  38.427  73.615  1.00 20.96           C
ANISOU 4813  C   LEU B  16     2692   2590   2680      6    -69     57       C
ATOM   4814  O   LEU B  16      65.574  39.653  73.604  1.00 21.14           O
ANISOU 4814  O   LEU B  16     2957   2456   2617    -27   -152    193       O
ATOM   4815  N   HIS B  17      64.642  37.855  74.637  1.00 19.82           N
ANISOU 4815  N   HIS B  17     2560   2374   2595    -38    -56     46       N
ATOM   4817  CA  HIS B  17      64.185  38.633  75.776  1.00 19.95           C
ANISOU 4817  CA  HIS B  17     2511   2435   2634    -17    -62     41       C
ATOM   4819  CB  HIS B  17      63.594  37.771  76.888  1.00 20.09           C
ANISOU 4819  CB  HIS B  17     2595   2471   2567      6    -52     77       C
ATOM   4822  CG  HIS B  17      62.173  37.362  76.665  1.00 23.15           C
ANISOU 4822  CG  HIS B  17     2775   2962   3057    -25    -61     67       C
ATOM   4823  ND1 HIS B  17      61.442  37.780  75.575  1.00 25.02           N
ANISOU 4823  ND1 HIS B  17     3252   3089   3165      8    -94    159       N
ATOM   4825  CE1 HIS B  17      60.188  37.387  75.734  1.00 25.92           C
ANISOU 4825  CE1 HIS B  17     3188   3272   3389   -107    -54    114       C
ATOM   4827  NE2 HIS B  17      60.159  36.496  76.714  1.00 25.98           N
ANISOU 4827  NE2 HIS B  17     3136   3367   3366   -140    -49     57       N
ATOM   4829  CD2 HIS B  17      61.409  36.421  77.279  1.00 24.62           C
ANISOU 4829  CD2 HIS B  17     3150   3052   3152    -65    -86    171       C
ATOM   4831  C   HIS B  17      65.412  39.382  76.317  1.00 18.59           C
ANISOU 4831  C   HIS B  17     2344   2255   2462     -8    -74      0       C
ATOM   4832  O   HIS B  17      66.510  38.835  76.288  1.00 18.10           O
ANISOU 4832  O   HIS B  17     2242   2080   2556   -107    -58     95       O
ATOM   4851  CB  ALA B  19      65.466  42.826  72.576  1.00 14.83           C
ANISOU 4851  CB  ALA B  19     1813   1767   2053   -157    -35    -55       C
ATOM   4855  C   ALA B  19      62.942  42.771  72.870  1.00 16.33           C
ANISOU 4855  C   ALA B  19     1931   2057   2215    -59    -79     62       C
ATOM   4856  O   ALA B  19      62.233  43.673  72.438  1.00 16.77           O
ANISOU 4856  O   ALA B  19     2027   1865   2480    -38    -88      4       O
ATOM   4857  N   THR B  20      62.568  41.500  72.794  1.00 16.98           N
ANISOU 4857  N   THR B  20     2123   2072   2254    -20   -143    -22       N
ATOM   4859  CA  THR B  20      61.257  41.119  72.214  1.00 18.21           C
ANISOU 4859  CA  THR B  20     2239   2345   2335    -35    -27    -16       C
ATOM   4861  CB  THR B  20      61.314  39.725  71.669  1.00 17.86           C
ANISOU 4861  CB  THR B  20     2209   2279   2298    -91     -7      2       C
ATOM   4863  OG1 THR B  20      61.904  38.854  72.642  1.00 17.92           O
ANISOU 4863  OG1 THR B  20     2537   2073   2197   -122   -174    -51       O
ATOM   4865  CG2 THR B  20      62.332  39.676  70.526  1.00 18.52           C
ANISOU 4865  CG2 THR B  20     2465   2331   2237   -110    122    -75       C
ATOM   4869  C   THR B  20      60.072  41.247  73.155  1.00 19.59           C
ANISOU 4869  C   THR B  20     2367   2545   2529    -34    -31     -9       C
ATOM   4870  O   THR B  20      59.005  40.734  72.852  1.00 18.68           O
ANISOU 4870  O   THR B  20     1946   2752   2397    -81    -23    -90       O
ATOM   4871  N   LEU B  21      60.262  41.859  74.313  1.00 20.51           N
ANISOU 4871  N   LEU B  21     2600   2632   2561    -11    -85    -72       N
ATOM   4873  CA  LEU B  21      59.119  42.158  75.148  1.00 22.04           C
ANISOU 4873  CA  LEU B  21     2713   2848   2811    -30      7    -18       C
ATOM   4900  N   ILE B  23      58.881  44.356  71.035  1.00 28.39           N
ANISOU 4900  N   ILE B  23     3571   3632   3581     78    -25    -57       N
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ATOM   4902  CA  ILE B  23      58.468  44.083  69.655  1.00 28.26           C
ANISOU 4902  CA  ILE B  23    3667   3572   3495     48    -45    -51       C
ATOM   4904  CB  ILE B  23      59.491  44.850  68.829  1.00 29.70           C
ANISOU 4904  CB  ILE B  23    3806   3766   3709     -4    -55    -30       C
ATOM   4906  CG1 ILE B  23      59.480  46.331  69.174  1.00 33.33           C
ANISOU 4906  CG1 ILE B  23    4333   4116   4215      5    -28     20       C
ATOM   4913  CG2 ILE B  23      59.309  44.662  67.361  1.00 31.12           C
ANISOU 4913  CG2 ILE B  23    3979   4049   3796      4    -34     46       C
ATOM   4917  C   ILE B  23      58.573  42.583  69.222  1.00 26.14           C
ANISOU 4917  C   ILE B  23    3361   3354   3217     83   -102    -65       C
ATOM   4918  O   ILE B  23      59.412  41.878  69.764  1.00 26.46           O
ANISOU 4918  O   ILE B  23    3613   3384   3054    167   -200    -74       O
ATOM   4919  N   SER B  24      57.781  42.124  68.223  1.00 22.94           N
ANISOU 4919  N   SER B  24    2867   2910   2936    146    -21    -55       N
ATOM   4921  CA  SER B  24      57.934  40.781  67.625  1.00 20.06           C
ANISOU 4921  CA  SER B  24    2483   2665   2472      1    -27     20       C
ATOM   4923  CB  SER B  24      56.993  40.556  66.420  1.00 20.18           C
ANISOU 4923  CB  SER B  24    2475   2606   2586    -27     29     14       C
ATOM   4926  OG  SER B  24      57.316  39.383  65.641  1.00 19.44           O
ANISOU 4926  OG  SER B  24    2256   2513   2616    210     85    116       O
ATOM   4928  C   SER B  24      59.353  40.734  67.107  1.00 17.16           C
ANISOU 4928  C   SER B  24    2132   2321   2066      8    -77    -46       C
ATOM   4929  O   SER B  24      59.856  41.739  66.618  1.00 15.55           O
ANISOU 4929  O   SER B  24    1769   2319   1818     57   -130   -193       O
ATOM   4930  N   LYS B  25      59.961  39.565  67.149  1.00 15.63           N
ANISOU 4930  N   LYS B  25    1859   2224   1854    -23    -54    -12       N
ATOM   4932  CA  LYS B  25      61.286  39.394  66.574  1.00 17.41           C
ANISOU 4932  CA  LYS B  25    2097   2301   2217    -35    -81      4       C
ATOM   4934  CB  LYS B  25      61.691  37.890  66.723  1.00 18.55           C
ANISOU 4934  CB  LYS B  25    2268   2376   2404     33    -62    -31       C
ATOM   4937  CG  LYS B  25      62.903  37.414  65.898  1.00 21.45           C
ANISOU 4937  CG  LYS B  25    2599   2829   2721    -54     73     -5       C
ATOM   4940  CD  LYS B  25      63.429  36.045  66.323  1.00 24.70           C
ANISOU 4940  CD  LYS B  25    2955   3220   3209     37    -12     86       C
ATOM   4943  CE  LYS B  25      62.583  34.836  66.028  1.00 26.45           C
ANISOU 4943  CE  LYS B  25    3461   3257   3330     55    -43    -81       C
ATOM   4946  NZ  LYS B  25      63.244  33.631  66.721  1.00 27.46           N
ANISOU 4946  NZ  LYS B  25    3550   3408   3476      9    -60     73       N
ATOM   4950  C   LYS B  25      61.277  39.851  65.103  1.00 16.13           C
ANISOU 4950  C   LYS B  25    1859   2213   2053    -65    -62     43       C
ATOM   4951  O   LYS B  25      62.225  40.491  64.603  1.00 17.01           O
ANISOU 4951  O   LYS B  25    1786   2328   2348   -117   -286     12       O
ATOM   4952  N   GLN B  26      60.172  39.607  64.393  1.00 14.29           N
ANISOU 4952  N   GLN B  26    1683   1850   1895    -99    -30    -42       N
ATOM   4954  CA  GLN B  26      60.135  39.935  62.967  1.00 12.33           C
ANISOU 4954  CA  GLN B  26    1412   1627   1645     -3     -2    -68       C
ATOM   4956  CB  GLN B  26      59.160  38.991  62.227  1.00 13.77           C
ANISOU 4956  CB  GLN B  26    1582   1815   1835    -54    -67     31       C
ATOM   4959  CG  GLN B  26      59.617  37.546  62.067  1.00 11.76           C
ANISOU 4959  CG  GLN B  26    1005   1916   1545    -26    334    -281       C
ATOM   4962  CD  GLN B  26      59.581  36.689  63.315  1.00 16.15           C
ANISOU 4962  CD  GLN B  26    2046   2170   1919    -41   -107    -222       C
ATOM   4963  OE1 GLN B  26      60.566  36.008  63.615  1.00 22.97           O
ANISOU 4963  OE1 GLN B  26    2888   2905   2932    273   -104    -351       O
ATOM   4964  NE2 GLN B  26      58.478  36.710  64.051  1.00 14.40           N
ANISOU 4964  NE2 GLN B  26    1690   2101   1678   -270    -82    -253       N
ATOM   4967  C   GLN B  26      59.904  41.406  62.600  1.00 12.55           C
ANISOU 4967  C   GLN B  26    1336   1821   1610    -28    -28     -8       C
ATOM   4968  O   GLN B  26      59.895  41.750  61.446  1.00 10.35           O
ANISOU 4968  O   GLN B  26     820   1519   1593     55      8    144       O
ATOM   4969  N   LEU B  27      59.665  42.252  63.599  1.00 12.42           N
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ANISOU 4969  N   LEU B  27     1476   1594   1645     73    -87    -57       N
ATOM   4971  CA  LEU B  27      59.570  43.668  63.386  1.00 14.13           C
ANISOU 4971  CA  LEU B  27     1761   1870   1737     -8    -24    -33       C
ATOM   4973  CB  LEU B  27      58.417  44.261  64.210  1.00 14.30           C
ANISOU 4973  CB  LEU B  27     1728   1828   1878     53      2     61       C
ATOM   4976  CG  LEU B  27      56.953  43.908  63.857  1.00 17.96           C
ANISOU 4976  CG  LEU B  27     2258   2430   2135   -119    -90    -45       C
ATOM   4978  CD1 LEU B  27      55.985  44.028  65.028  1.00 19.08           C
ANISOU 4978  CD1 LEU B  27     2174   2447   2626    122     78    -26       C
ATOM   4982  CD2 LEU B  27      56.513  44.848  62.793  1.00 22.11           C
ANISOU 4982  CD2 LEU B  27     2759   2721   2921      2   -188    170       C
ATOM   4986  C   LEU B  27      60.891  44.309  63.775  1.00 14.03           C
ANISOU 4986  C   LEU B  27     1766   1801   1763      1     55    -12       C
ATOM   4987  O   LEU B  27      61.067  45.442  63.475  1.00 17.04           O
ANISOU 4987  O   LEU B  27     2240   2003   2228    -14     -5    -49       O
ATOM   4988  N   LEU B  28      61.835  43.599  64.409  1.00 14.02           N
ANISOU 4988  N   LEU B  28     1660   1909   1756    -90     22     13       N
ATOM   4990  CA  LEU B  28      63.150  44.224  64.778  1.00 13.99           C
ANISOU 4990  CA  LEU B  28     1700   1844   1770    -48     28     -6       C
ATOM   4992  CB  LEU B  28      63.975  43.297  65.652  1.00 14.06           C
ANISOU 4992  CB  LEU B  28     1569   1932   1840    -71     -4     28       C
ATOM   4995  CG  LEU B  28      63.284  42.777  66.926  1.00 16.82           C
ANISOU 4995  CG  LEU B  28     2083   2235   2070    -22     15    -12       C
ATOM   4997  CD1 LEU B  28      64.143  41.766  67.650  1.00 17.68           C
ANISOU 4997  CD1 LEU B  28     2269   2266   2183     29    -66    -47       C
ATOM   5001  CD2 LEU B  28      62.938  43.956  67.787  1.00 17.08           C
ANISOU 5001  CD2 LEU B  28     2064   2215   2209    -97     30   -130       C
ATOM   5005  C   LEU B  28      63.959  44.497  63.522  1.00 12.02           C
ANISOU 5005  C   LEU B  28     1390   1585   1593     -9    -12     -1       C
ATOM   5006  O   LEU B  28      63.867  43.764  62.571  1.00 11.97           O
ANISOU 5006  O   LEU B  28     1322   1608   1617   -216   -266    -58       O
ATOM   5007  N   PRO B  29      64.797  45.511  63.514  1.00 11.04           N
ANISOU 5007  N   PRO B  29     1405   1409   1380    -60     -6    -23       N
ATOM   5008  CA  PRO B  29      65.582  45.786  62.322  1.00 10.79           C
ANISOU 5008  CA  PRO B  29     1354   1313   1432    -38     40    -46       C
ATOM   5016  CD  PRO B  29      65.040  46.471  64.594  1.00 12.34           C
ANISOU 5016  CD  PRO B  29     1490   1521   1677    -86    126      1       C
ATOM   5019  C   PRO B  29      66.733  44.847  62.108  1.00 10.21           C
ANISOU 5019  C   PRO B  29     1336   1214   1326    -11      5    -31       C
ATOM   5020  O   PRO B  29      67.323  44.363  63.089  1.00  9.91           O
ANISOU 5020  O   PRO B  29     1459   1088   1217   -101      2    -85       O
ATOM   5021  N   VAL B  30      67.017  44.568  60.839  1.00  9.27           N
ANISOU 5021  N   VAL B  30     1201   1105   1215     19     60     77       N
ATOM   5023  CA  VAL B  30      68.303  43.966  60.479  1.00  8.71           C
ANISOU 5023  CA  VAL B  30     1083   1091   1134    -18    -15     23       C
ATOM   5025  CB  VAL B  30      68.168  42.703  59.648  1.00  8.93           C
ANISOU 5025  CB  VAL B  30     1171    959   1263     35     59     70       C
ATOM   5027  CG1 VAL B  30      69.520  42.182  59.238  1.00 10.43           C
ANISOU 5027  CG1 VAL B  30     1330   1166   1465    -81     65    -35       C
ATOM   5031  CG2 VAL B  30      67.318  41.657  60.445  1.00  9.24           C
ANISOU 5031  CG2 VAL B  30     1205   1183   1120    128     15    197       C
ATOM   5035  C   VAL B  30      68.991  45.071  59.707  1.00  7.93           C
ANISOU 5035  C   VAL B  30     920   1043   1050     39      4     10       C
ATOM   5090  C   LYS B  33      64.361  46.616  58.455  1.00  8.34           C
ANISOU 5090  C   LYS B  33     929    974   1263    -11    -12    -84       C
ATOM   5091  O   LYS B  33      65.113  45.827  58.991  1.00  9.24           O
ANISOU 5091  O   LYS B  33     781   1411   1315   -102    -25    -87       O
ATOM   5092  N   PRO B  34      63.047  46.558  58.667  1.00  7.59           N
ANISOU 5092  N   PRO B  34     970    818   1094    -84      4   -105       N
ATOM   5093  CA  PRO B  34      62.472  45.513  59.507  1.00  8.98           C
ANISOU 5093  CA  PRO B  34     1077   1182   1152    -23     35    -39       C
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ATOM   5095  CB  PRO B  34      60.985  45.768  59.400  1.00  9.13           C
ANISOU 5095  CB  PRO B  34    1067   1116   1285    -48    23     62       C
ATOM   5098  CG  PRO B  34      60.849  47.252  59.081  1.00 10.63           C
ANISOU 5098  CG  PRO B  34    1298   1261   1479   -145    35     21       C
ATOM   5104  C   PRO B  34      62.771  44.107  59.005  1.00  7.71           C
ANISOU 5104  C   PRO B  34     816    983   1128    -25    -1     -9       C
ATOM   5105  O   PRO B  34      62.764  43.847  57.773  1.00  7.91           O
ANISOU 5105  O   PRO B  34     713   1166   1125    111    81     -8       O
ATOM   5106  N   MET B  35      63.017  43.207  59.951  1.00  7.63           N
ANISOU 5106  N   MET B  35     706   1152   1039   -122    87    -32       N
ATOM   5108  CA  MET B  35      63.328  41.808  59.621  1.00  9.13           C
ANISOU 5108  CA  MET B  35    1145   1167   1154    -49     7    -19       C
ATOM   5110  CB  MET B  35      63.300  40.920  60.858  1.00  9.98           C
ANISOU 5110  CB  MET B  35    1300   1325   1166    -82    11     -5       C
ATOM   5113  CG  MET B  35      63.864  39.465  60.653  1.00 11.02           C
ANISOU 5113  CG  MET B  35    1780   1158   1246   -345  -175   -105       C
ATOM   5116  SD  MET B  35      63.800  38.601  62.205  1.00 14.63           S
ANISOU 5116  SD  MET B  35    1523   2283   1753   -297    95    121       S
ATOM   5117  CE  MET B  35      64.826  39.520  63.177  1.00 15.95           C
ANISOU 5117  CE  MET B  35    2042   2110   1907   -184   -25     83       C
ATOM   5121  C   MET B  35      62.385  41.213  58.575  1.00  8.72           C
ANISOU 5121  C   MET B  35    1112   1140   1059    -50    19      1       C
ATOM   5122  O   MET B  35      62.867  40.538  57.670  1.00  8.66           O
ANISOU 5122  O   MET B  35    1201   1148    939    -13     2    -84       O
ATOM   5123  N   ILE B  36      61.076  41.436  58.713  1.00  8.24           N
ANISOU 5123  N   ILE B  36    1075   1059    993    -10    76     -1       N
ATOM   5125  CA  ILE B  36      60.102  40.883  57.768  1.00  8.01           C
ANISOU 5125  CA  ILE B  36     872   1072   1097     33    47     58       C
ATOM   5127  CB  ILE B  36      58.619  41.164  58.237  1.00  9.39           C
ANISOU 5127  CB  ILE B  36    1145   1265   1155     -1    83    -47       C
ATOM   5129  CG1 ILE B  36      57.741  40.087  57.611  1.00 11.66           C
ANISOU 5129  CG1 ILE B  36    1333   1657   1439    -49   -24   -111       C
ATOM   5132  CD1 ILE B  36      56.387  39.965  58.155  1.00 12.01           C
ANISOU 5132  CD1 ILE B  36    1482   1729   1350   -188    -7    -57       C
ATOM   5136  CG2 ILE B  36      58.183  42.568  57.920  1.00 11.74           C
ANISOU 5136  CG2 ILE B  36    1296   1644   1519     37   -37     -4       C
ATOM   5140  C   ILE B  36      60.336  41.218  56.285  1.00  7.69           C
ANISOU 5140  C   ILE B  36     853    973   1095     -6    66    -32       C
ATOM   5141  O   ILE B  36      59.901  40.475  55.413  1.00  8.24           O
ANISOU 5141  O   ILE B  36    1146    904   1080   -148   207     56       O
ATOM   5142  N   TYR B  37      60.947  42.386  55.989  1.00  7.41           N
ANISOU 5142  N   TYR B  37     862   1008    946     -3   113      2       N
ATOM   5144  CA  TYR B  37      61.314  42.718  54.635  1.00  6.57           C
ANISOU 5144  CA  TYR B  37     834    832    831      5    12     41       C
ATOM   5146  CB  TYR B  37      62.094  44.051  54.598  1.00  5.76           C
ANISOU 5146  CB  TYR B  37     671    937    580     20   126    -78       C
ATOM   5149  CG  TYR B  37      61.225  45.319  54.625  1.00  6.27           C
ANISOU 5149  CG  TYR B  37     763    977    640     79   -53    138       C
ATOM   5150  CD1 TYR B  37      59.977  45.362  55.285  1.00  6.67           C
ANISOU 5150  CD1 TYR B  37     689    923    922   -116  -212    178       C
ATOM   5161  C   TYR B  37      62.118  41.618  53.938  1.00  6.40           C
ANISOU 5161  C   TYR B  37     667    847    916   -119    69     37       C
ATOM   5162  O   TYR B  37      61.976  41.379  52.731  1.00  5.51           O
ANISOU 5162  O   TYR B  37     528    726    839    -18   104    -29       O
ATOM   5163  N   TYR B  38      62.957  40.932  54.685  1.00  6.74           N
ANISOU 5163  N   TYR B  38     940    848    772   -144    38     31       N
ATOM   5165  CA  TYR B  38      63.881  39.967  54.092  1.00  8.02           C
ANISOU 5165  CA  TYR B  38     992   1023   1029     -5    38      1       C
ATOM   5167  CB  TYR B  38      65.067  39.689  55.038  1.00  8.26           C
ANISOU 5167  CB  TYR B  38    1020   1040   1077    -34   123    -31       C
ATOM   5170  CG  TYR B  38      65.918  40.911  55.307  1.00  6.50           C
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ANISOU	5170	CG	TYR	B	38	695	1064	710	127	-40	61		C
ATOM	5171	CD1	TYR	B	38	65.620	41.760	56.335	1.00	7.59			C
ANISOU	5171	CD1	TYR	B	38	1037	774	1070	44	-9	102		C
ATOM	5173	CE1	TYR	B	38	66.380	42.897	56.588	1.00	7.58			C
ANISOU	5173	CE1	TYR	B	38	754	1048	1077	84	-110	30		C
ATOM	5175	CZ	TYR	B	38	67.516	43.123	55.821	1.00	8.57			C
ANISOU	5175	CZ	TYR	B	38	1206	1091	960	-116	145	-54		C
ATOM	5178	CE2	TYR	B	38	67.850	42.266	54.797	1.00	10.12			C
ANISOU	5178	CE2	TYR	B	38	1517	1163	1162	41	187	-86		C
ATOM	5180	CD2	TYR	B	38	67.048	41.181	54.534	1.00	9.81			C
ANISOU	5180	CD2	TYR	B	38	1027	1419	1280	-148	71	51		C
ATOM	5182	C	TYR	B	38	63.124	38.704	53.553	1.00	9.16			C
ANISOU	5182	C	TYR	B	38	1277	1001	1200	-16	64	-2		C
ATOM	5183	O	TYR	B	38	63.177	38.411	52.348	1.00	8.72			O
ANISOU	5183	O	TYR	B	38	1364	836	1111	184	121	0		O
ATOM	5184	N	PRO	B	39	62.338	37.999	54.378	1.00	9.47			N
ANISOU	5184	N	PRO	B	39	1333	1130	1135	-73	61	1		N
ATOM	5185	CA	PRO	B	39	61.552	36.872	53.837	1.00	9.40			C
ANISOU	5185	CA	PRO	B	39	1217	1157	1197	-69	12	-31		C
ATOM	5187	CB	PRO	B	39	60.966	36.211	55.091	1.00	8.17			C
ANISOU	5187	CB	PRO	B	39	970	1021	1114	18	-26	-59		C
ATOM	5190	CG	PRO	B	39	60.977	37.302	56.148	1.00	8.67			C
ANISOU	5190	CG	PRO	B	39	1240	1077	974	-89	-81	63		C
ATOM	5193	CD	PRO	B	39	62.242	38.067	55.845	1.00	10.35			C
ANISOU	5193	CD	PRO	B	39	1374	1284	1274	-114	45	-67		C
ATOM	5196	C	PRO	B	39	60.469	37.287	52.801	1.00	9.44			C
ANISOU	5196	C	PRO	B	39	1156	1145	1285	-8	35	13		C
ATOM	5197	O	PRO	B	39	60.149	36.501	51.862	1.00	9.58			O
ANISOU	5197	O	PRO	B	39	1047	1048	1541	22	-9	12		O
ATOM	5198	N	LEU	B	40	59.917	38.495	52.964	1.00	8.59			N
ANISOU	5198	N	LEU	B	40	1006	1121	1136	-54	144	60		N
ATOM	5200	CA	LEU	B	40	58.945	39.015	52.060	1.00	8.88			C
ANISOU	5200	CA	LEU	B	40	1124	1117	1132	-19	92	67		C
ATOM	5202	CB	LEU	B	40	58.462	40.389	52.565	1.00	8.20			C
ANISOU	5202	CB	LEU	B	40	1099	1127	888	-26	95	36		C
ATOM	5205	CG	LEU	B	40	57.606	41.124	51.517	1.00	10.43			C
ANISOU	5205	CG	LEU	B	40	1296	1268	1398	23	36	10		C
ATOM	5207	CD1	LEU	B	40	56.432	40.286	51.194	1.00	12.24			C
ANISOU	5207	CD1	LEU	B	40	1421	1546	1683	72	109	-192		C
ATOM	5211	CD2	LEU	B	40	57.186	42.500	51.998	1.00	10.51			C
ANISOU	5211	CD2	LEU	B	40	1163	1479	1348	32	-25	-2		C
ATOM	5215	C	LEU	B	40	59.616	39.162	50.677	1.00	9.80			C
ANISOU	5215	C	LEU	B	40	1282	1260	1180	84	11	26		C
ATOM	5216	O	LEU	B	40	59.108	38.692	49.649	1.00	8.59			O
ANISOU	5216	O	LEU	B	40	1091	1004	1167	245	-53	-19		O
ATOM	5217	N	SER	B	41	60.791	39.769	50.695	1.00	10.05			N
ANISOU	5217	N	SER	B	41	1352	1208	1258	-22	6	37		N
ATOM	5219	CA	SER	B	41	61.610	39.892	49.501	1.00	10.26			C
ANISOU	5219	CA	SER	B	41	1399	1306	1194	78	5	0		C
ATOM	5224	OG	SER	B	41	64.043	39.812	50.309	1.00	12.34			O
ANISOU	5224	OG	SER	B	41	1173	1758	1757	-134	-105	-71		O
ATOM	5226	C	SER	B	41	61.897	38.523	48.816	1.00	10.05			C
ANISOU	5226	C	SER	B	41	1325	1231	1263	26	-2	0		C
ATOM	5228	N	THR	B	42	62.099	37.494	49.625	1.00	8.33			N
ANISOU	5228	N	THR	B	42	985	1187	991	1	63	17		N
ATOM	5230	CA	THR	B	42	62.379	36.162	49.122	1.00	8.14			C
ANISOU	5230	CA	THR	B	42	907	1146	1040	-54	52	-17		C
ATOM	5232	CB	THR	B	42	62.784	35.260	50.254	1.00	8.33			C
ANISOU	5232	CB	THR	B	42	869	1263	1033	5	19	-75		C
ATOM	5234	OG1	THR	B	42	64.133	35.579	50.714	1.00	9.46			O
ANISOU	5234	OG1	THR	B	42	873	1479	1239	32	-198	-150		O

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ATOM   5236  CG2 THR B  42      62.799  33.833  49.839  1.00  9.75           C
ANISOU 5236  CG2 THR B  42    1166   1363   1174    -27     23    105       C
ATOM   5240  C   THR B  42      61.167  35.625  48.327  1.00  8.32           C
ANISOU 5240  C   THR B  42     991   1127   1041    -50     44     12       C
ATOM   5242  N   LEU B  43      59.992  35.709  48.907  1.00  8.39           N
ANISOU 5242  N   LEU B  43     984   1047   1156     47     82     37       N
ATOM   5244  CA  LEU B  43      58.798  35.361  48.143  1.00  7.89           C
ANISOU 5244  CA  LEU B  43    1050    962    987    -17     47    -52       C
ATOM   5246  CB  LEU B  43      57.575  35.459  49.014  1.00  7.75           C
ANISOU 5246  CB  LEU B  43     886    945   1113     77     64    -85       C
ATOM   5249  CG  LEU B  43      57.550  34.563  50.258  1.00  8.26           C
ANISOU 5249  CG  LEU B  43     874   1120   1143     -6      1    -27       C
ATOM   5251  CD1 LEU B  43      56.172  34.819  50.988  1.00 10.56           C
ANISOU 5251  CD1 LEU B  43    1282   1449   1281    -46    130    -24       C
ATOM   5255  CD2 LEU B  43      57.674  33.086  49.916  1.00 10.22           C
ANISOU 5255  CD2 LEU B  43    1340   1421   1120     88     74     -2       C
ATOM   5374  CA  ILE B  51      51.084  36.450  50.452  1.00  7.96           C
ANISOU 5374  CA  ILE B  51     949    989   1085      9     41     31       C
ATOM   5376  CB  ILE B  51      52.425  37.184  50.586  1.00  8.70           C
ANISOU 5376  CB  ILE B  51    1184    996   1124     38     33    -22       C
ATOM   5385  CG2 ILE B  51      53.101  36.831  51.886  1.00  9.88           C
ANISOU 5385  CG2 ILE B  51    1051   1327   1375    -98    108     59       C
ATOM   5389  C   ILE B  51      50.267  36.649  51.721  1.00  8.56           C
ANISOU 5389  C   ILE B  51    1107   1075   1070    105    -24    -22       C
ATOM   5390  O   ILE B  51      49.738  37.768  52.001  1.00  8.21           O
ANISOU 5390  O   ILE B  51    1080   1144    894    210   -106    -81       O
ATOM   5391  N   LEU B  52      50.161  35.569  52.484  1.00  8.46           N
ANISOU 5391  N   LEU B  52     912   1127   1172     85     10     -8       N
ATOM   5393  CA  LEU B  52      49.565  35.575  53.807  1.00  8.24           C
ANISOU 5393  CA  LEU B  52    1001   1062   1067     40     24      6       C
ATOM   5395  CB  LEU B  52      48.754  34.291  53.982  1.00  8.67           C
ANISOU 5395  CB  LEU B  52    1178   1014   1101     77     57     18       C
ATOM   5398  CG  LEU B  52      48.054  34.060  55.339  1.00  7.53           C
ANISOU 5398  CG  LEU B  52     927   1041    892     33    -43      8       C
ATOM   5400  CD1 LEU B  52      46.944  35.069  55.573  1.00  8.59           C
ANISOU 5400  CD1 LEU B  52    1101   1105   1056    -86    337     62       C
ATOM   5404  CD2 LEU B  52      47.521  32.680  55.511  1.00  8.31           C
ANISOU 5404  CD2 LEU B  52     960   1189   1008    166     49   -134       C
ATOM   5408  C   LEU B  52      50.635  35.654  54.883  1.00  8.13           C
ANISOU 5408  C   LEU B  52     999    958   1129     19     70     10       C
ATOM   5409  O   LEU B  52      51.626  34.852  54.886  1.00  9.12           O
ANISOU 5409  O   LEU B  52    1034   1130   1300    294     32     -3       O
ATOM   5410  N   ILE B  53      50.484  36.634  55.776  1.00  7.32           N
ANISOU 5410  N   ILE B  53     919    990    871     71    131     43       N
ATOM   5412  CA  ILE B  53      51.421  36.851  56.886  1.00  7.74           C
ANISOU 5412  CA  ILE B  53     977    964    997     38     86     27       C
ATOM   5414  CB  ILE B  53      51.817  38.309  56.986  1.00  8.49           C
ANISOU 5414  CB  ILE B  53    1166   1046   1013     -6     30    -30       C
ATOM   5416  CG1 ILE B  53      52.598  38.707  55.730  1.00 10.63           C
ANISOU 5416  CG1 ILE B  53    1234   1289   1512    -14     90    100       C
ATOM   5419  CD1 ILE B  53      52.807  40.069  55.625  1.00 13.20           C
ANISOU 5419  CD1 ILE B  53    1748   1539   1726    -85    202      1       C
ATOM   5423  CG2 ILE B  53      52.616  38.568  58.211  1.00  8.69           C
ANISOU 5423  CG2 ILE B  53    1074   1006   1221     12    -70     24       C
ATOM   5427  C   ILE B  53      50.725  36.389  58.134  1.00  7.77           C
ANISOU 5427  C   ILE B  53    1021   1001    929     35     49    -30       C
ATOM   5428  O   ILE B  53      49.630  36.892  58.492  1.00  7.32           O
ANISOU 5428  O   ILE B  53     928    969    883    -11      2     81       O
ATOM   5429  N   ILE B  54      51.310  35.350  58.720  1.00  8.14           N
ANISOU 5429  N   ILE B  54     911   1174   1005     38     39     45       N
ATOM   5431  CA  ILE B  54      50.812  34.787  59.936  1.00  9.27           C
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ANISOU	5431	CA	ILE	B	54	1091	1292	1136	2	61	15		C
ATOM	5433	CB	ILE	B	54	50.743	33.260	59.869	1.00	8.45			C
ANISOU	5433	CB	ILE	B	54	997	1241	970	-9	137	-23		C
ATOM	5435	CG1	ILE	B	54	49.809	32.847	58.725	1.00	9.41			C
ANISOU	5435	CG1	ILE	B	54	1015	1221	1339	34	5	99		C
ATOM	5438	CD1	ILE	B	54	49.762	31.413	58.454	1.00	9.26			C
ANISOU	5438	CD1	ILE	B	54	1132	1327	1056	-31	23	32		C
ATOM	5442	CG2	ILE	B	54	50.268	32.690	61.194	1.00	8.94			C
ANISOU	5442	CG2	ILE	B	54	1254	1152	991	-81	74	-158		C
ATOM	5446	C	ILE	B	54	51.628	35.258	61.121	1.00	9.49			C
ANISOU	5446	C	ILE	B	54	1065	1318	1222	-31	14	0		C
ATOM	5447	O	ILE	B	54	52.850	35.189	61.105	1.00	10.96			O
ANISOU	5447	O	ILE	B	54	1177	1581	1406	146	108	-47		O
ATOM	5448	N	SER	B	55	50.942	35.752	62.147	1.00	8.46			N
ANISOU	5448	N	SER	B	55	948	1105	1162	3	-25	-34		N
ATOM	5450	CA	SER	B	55	51.604	36.172	63.361	1.00	8.73			C
ANISOU	5450	CA	SER	B	55	1070	1142	1104	70	-16	40		C
ATOM	5452	CB	SER	B	55	52.151	37.586	63.282	1.00	8.67			C
ANISOU	5452	CB	SER	B	55	1042	1193	1058	-1	42	37		C
ATOM	5455	OG	SER	B	55	53.131	37.809	64.325	1.00	13.77			O
ANISOU	5455	OG	SER	B	55	1638	1951	1640	260	-4	-247		O
ATOM	5457	C	SER	B	55	50.729	35.916	64.604	1.00	8.11			C
ANISOU	5457	C	SER	B	55	834	1177	1068	71	59	-85		C
ATOM	5458	O	SER	B	55	49.690	35.226	64.541	1.00	7.60			O
ANISOU	5458	O	SER	B	55	765	1202	921	198	-149	-9		O
ATOM	5459	N	THR	B	56	51.268	36.289	65.740	1.00	8.14			N
ANISOU	5459	N	THR	B	56	747	1172	1170	-27	3	-68		N
ATOM	5461	CA	THR	B	56	50.593	36.155	66.977	1.00	8.46			C
ANISOU	5461	CA	THR	B	56	993	1166	1052	-59	-3	-4		C
ATOM	5463	CB	THR	B	56	51.456	36.546	68.219	1.00	8.45			C
ANISOU	5463	CB	THR	B	56	837	1109	1261	-48	-17	-13		C
ATOM	5465	OG1	THR	B	56	51.823	37.916	68.140	1.00	8.18			O
ANISOU	5465	OG1	THR	B	56	673	1239	1193	-211	14	-72		O
ATOM	5467	CG2	THR	B	56	52.690	35.717	68.381	1.00	8.38			C
ANISOU	5467	CG2	THR	B	56	896	1123	1165	-50	-166	54		C
ATOM	5471	C	THR	B	56	49.396	37.092	67.002	1.00	8.49			C
ANISOU	5471	C	THR	B	56	835	1182	1207	13	-73	20		C
ATOM	5472	O	THR	B	56	49.310	38.055	66.229	1.00	9.15			O
ANISOU	5472	O	THR	B	56	870	1418	1188	-94	72	-13		O
ATOM	5473	N	PRO	B	57	48.475	36.899	67.924	1.00	9.92			N
ANISOU	5473	N	PRO	B	57	1184	1287	1296	1	5	40		N
ATOM	5474	CA	PRO	B	57	47.374	37.862	67.966	1.00	10.34			C
ANISOU	5474	CA	PRO	B	57	1147	1341	1437	-22	2	47		C
ATOM	5476	CB	PRO	B	57	46.468	37.335	69.114	1.00	10.65			C
ANISOU	5476	CB	PRO	B	57	1334	1382	1329	47	70	9		C
ATOM	5479	CG	PRO	B	57	46.849	35.898	69.207	1.00	12.15			C
ANISOU	5479	CG	PRO	B	57	1646	1516	1454	-80	112	88		C
ATOM	5482	CD	PRO	B	57	48.269	35.810	68.893	1.00	10.25			C
ANISOU	5482	CD	PRO	B	57	1179	1238	1476	87	-110	0		C
ATOM	5485	C	PRO	B	57	47.793	39.276	68.226	1.00	10.09			C
ANISOU	5485	C	PRO	B	57	1130	1350	1350	26	92	2		C
ATOM	5486	O	PRO	B	57	47.269	40.136	67.586	1.00	9.04			O
ANISOU	5486	O	PRO	B	57	950	1294	1189	-240	-42	135		O
ATOM	5487	N	GLN	B	58	48.770	39.505	69.092	1.00	11.87			N
ANISOU	5487	N	GLN	B	58	1525	1550	1434	55	-19	-26		N
ATOM	5489	CA	GLN	B	58	49.196	40.862	69.443	1.00	14.41			C
ANISOU	5489	CA	GLN	B	58	1816	1859	1799	13	-11	-6		C
ATOM	5491	CB	GLN	B	58	49.987	40.857	70.796	1.00	15.87			C
ANISOU	5491	CB	GLN	B	58	1992	2028	2007	42	-94	0		C
ATOM	5494	CG	GLN	B	58	51.339	40.228	70.688	1.00	19.01			C
ANISOU	5494	CG	GLN	B	58	2329	2467	2424	116	-5	42		C

ATOM	5497	CD	GLN	B	58	51.329	38.693	71.012	1.00	23.61		C
ANISOU	5497	CD	GLN	B	58	3019	2751	3200	-19	-33	94	C
ATOM	5498	OE1	GLN	B	58	50.245	38.016	70.990	1.00	22.34		O
ANISOU	5498	OE1	GLN	B	58	2795	3342	2348	-67	121	-19	O
ATOM	5499	NE2	GLN	B	58	52.549	38.137	71.275	1.00	23.63		N
ANISOU	5499	NE2	GLN	B	58	2829	3109	3038	41	-165	-25	N
ATOM	5502	C	GLN	B	58	50.036	41.528	68.370	1.00	13.95		C
ANISOU	5502	C	GLN	B	58	1667	1803	1827	13	6	19	C
ATOM	5503	O	GLN	B	58	50.089	42.735	68.288	1.00	14.86		O
ANISOU	5503	O	GLN	B	58	1794	1858	1992	76	103	16	O
ATOM	5504	N	ASP	B	59	50.712	40.742	67.553	1.00	14.39		N
ANISOU	5504	N	ASP	B	59	1845	1836	1785	-15	-5	-14	N
ATOM	5506	CA	ASP	B	59	51.645	41.332	66.575	1.00	13.88		C
ANISOU	5506	CA	ASP	B	59	1774	1710	1789	7	33	-22	C
ATOM	5508	CB	ASP	B	59	52.874	40.486	66.413	1.00	13.83		C
ANISOU	5508	CB	ASP	B	59	1677	1809	1768	-22	29	-25	C
ATOM	5511	CG	ASP	B	59	53.709	40.483	67.649	1.00	17.18		C
ANISOU	5511	CG	ASP	B	59	2013	2276	2238	-75	-176	35	C
ATOM	5512	OD1	ASP	B	59	54.145	41.604	68.007	1.00	19.30		O
ANISOU	5512	OD1	ASP	B	59	2295	2293	2746	239	-275	-218	O
ATOM	5513	OD2	ASP	B	59	53.944	39.422	68.309	1.00	16.82		O
ANISOU	5513	OD2	ASP	B	59	1632	2429	2330	-89	-408	59	O
ATOM	5514	C	ASP	B	59	51.008	41.507	65.255	1.00	13.43		C
ANISOU	5514	C	ASP	B	59	1681	1742	1680	42	52	-44	C
ATOM	5515	O	ASP	B	59	51.442	42.288	64.465	1.00	13.54		O
ANISOU	5515	O	ASP	B	59	1813	1634	1695	46	-31	64	O
ATOM	5516	N	THR	B	60	49.962	40.762	65.009	1.00	14.48		N
ANISOU	5516	N	THR	B	60	1928	1872	1701	-27	69	-69	N
ATOM	5518	CA	THR	B	60	49.296	40.874	63.715	1.00	15.28		C
ANISOU	5518	CA	THR	B	60	1925	2036	1841	-13	-17	-4	C
ATOM	5520	CB	THR	B	60	48.065	39.976	63.649	1.00	15.25		C
ANISOU	5520	CB	THR	B	60	1890	2040	1863	-1	33	-67	C
ATOM	5522	OG1	THR	B	60	48.416	38.583	63.562	1.00	15.64		O
ANISOU	5522	OG1	THR	B	60	1672	2323	1948	-52	-2	8	O
ATOM	5524	CG2	THR	B	60	47.327	40.272	62.352	1.00	15.83		C
ANISOU	5524	CG2	THR	B	60	1941	2113	1962	-58	-82	52	C
ATOM	5528	C	THR	B	60	48.946	42.335	63.323	1.00	15.48		C
ANISOU	5528	C	THR	B	60	2032	1957	1890	-43	2	-80	C
ATOM	5529	O	THR	B	60	49.275	42.805	62.216	1.00	15.73		O
ANISOU	5529	O	THR	B	60	2196	2032	1748	-86	67	-79	O
ATOM	5530	N	PRO	B	61	48.339	43.108	64.204	1.00	15.22		N
ANISOU	5530	N	PRO	B	61	1873	2044	1865	-14	113	2	N
ATOM	5531	CA	PRO	B	61	48.018	44.498	63.847	1.00	15.29		C
ANISOU	5531	CA	PRO	B	61	1906	1998	1904	28	73	-21	C
ATOM	5536	CG	PRO	B	61	46.840	43.719	65.774	1.00	15.26		C
ANISOU	5536	CG	PRO	B	61	1788	2061	1946	37	119	28	C
ATOM	5539	CD	PRO	B	61	47.910	42.752	65.559	1.00	16.01		C
ANISOU	5539	CD	PRO	B	61	2094	2027	1959	-3	-2	-1	C
ATOM	5542	C	PRO	B	61	49.270	45.361	63.602	1.00	15.54		C
ANISOU	5542	C	PRO	B	61	1936	2023	1945	84	85	-39	C
ATOM	5544	N	ARG	B	62	50.386	44.953	64.170	1.00	15.87		N
ANISOU	5544	N	ARG	B	62	1985	2129	1914	55	6	-9	N
ATOM	5546	CA	ARG	B	62	51.613	45.727	63.973	1.00	15.78		C
ANISOU	5546	CA	ARG	B	62	1973	2019	2001	34	63	-23	C
ATOM	5548	CB	ARG	B	62	52.648	45.354	65.012	1.00	16.56		C
ANISOU	5548	CB	ARG	B	62	2052	2145	2093	-33	16	-42	C
ATOM	5551	CG	ARG	B	62	52.135	45.380	66.432	1.00	21.36		C
ANISOU	5551	CG	ARG	B	62	2819	2687	2609	0	44	-15	C
ATOM	5554	CD	ARG	B	62	53.207	45.355	67.475	1.00	24.85		C
ANISOU	5554	CD	ARG	B	62	3140	3144	3157	-68	-140	59	C
ATOM	5557	NE	ARG	B	62	52.576	45.498	68.786	1.00	29.42		N

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ANISOU 5557  NE  ARG B  62     3763   3767   3648     90     81    -43       N
ATOM   5559  CZ  ARG B  62      52.591  44.583  69.758  1.00 31.69           C
ANISOU 5559  CZ  ARG B  62     4093   3979   3967    -32     -2     55       C
ATOM   5560  NH1 ARG B  62      53.245  43.426  69.621  1.00 31.75           N
ANISOU 5560  NH1 ARG B  62     3953   4091   4019     57     -2     85       N
ATOM   5566  C   ARG B  62      52.138  45.467  62.552  1.00 15.23           C
ANISOU 5566  C   ARG B  62     1861   1997   1928      9    -39     16       C
ATOM   5567  O   ARG B  62      52.666  46.357  61.875  1.00 14.60           O
ANISOU 5567  O   ARG B  62     1885   1838   1824    138      3     49       O
ATOM   5568  N   PHE B  63      52.032  44.239  62.103  1.00 14.42           N
ANISOU 5568  N   PHE B  63     1762   1881   1835     24      1    -30       N
ATOM   5570  CA  PHE B  63      52.434  43.988  60.730  1.00 14.37           C
ANISOU 5570  CA  PHE B  63     1812   1847   1800    -26     39     61       C
ATOM   5572  CB  PHE B  63      52.532  42.512  60.442  1.00 14.23           C
ANISOU 5572  CB  PHE B  63     1706   1816   1884    -38     61     44       C
ATOM   5575  CG  PHE B  63      53.669  41.851  61.120  1.00 14.00           C
ANISOU 5575  CG  PHE B  63     1775   1805   1737    -67     10     35       C
ATOM   5576  CD1 PHE B  63      53.469  41.123  62.270  1.00 14.72           C
ANISOU 5576  CD1 PHE B  63     1913   1808   1871    238    179     81       C
ATOM   5578  CE1 PHE B  63      54.507  40.516  62.917  1.00 15.76           C
ANISOU 5578  CE1 PHE B  63     1851   2147   1989   -150    -35    188       C
ATOM   5580  CZ  PHE B  63      55.765  40.618  62.449  1.00 15.25           C
ANISOU 5580  CZ  PHE B  63     1838   2072   1884    221    176    118       C
ATOM   5582  CE2 PHE B  63      55.992  41.391  61.319  1.00 18.17           C
ANISOU 5582  CE2 PHE B  63     2331   2417   2152    171    127    222       C
ATOM   5584  CD2 PHE B  63      54.932  41.983  60.644  1.00 14.15           C
ANISOU 5584  CD2 PHE B  63     1678   2026   1671     93    118     94       C
ATOM   5586  C   PHE B  63      51.458  44.678  59.758  1.00 13.76           C
ANISOU 5586  C   PHE B  63     1674   1784   1768      1     32     47       C
ATOM   5587  O   PHE B  63      51.861  45.219  58.719  1.00 12.02           O
ANISOU 5587  O   PHE B  63     1667   1384   1514    -27     74     96       O
ATOM   5588  N   GLN B  64      50.170  44.624  60.060  1.00 13.88           N
ANISOU 5588  N   GLN B  64     1702   1766   1804     27     73     19       N
ATOM   5635  CD2 LEU B  66      57.020  46.274  58.876  1.00 14.82           C
ANISOU 5635  CD2 LEU B  66     1778   1960   1890      0   -109    122       C
ATOM   5648  CG  LEU B  67      54.382  44.799  55.922  1.00 13.29           C
ANISOU 5648  CG  LEU B  67     1725   1771   1552    -68     22     33       C
ATOM   5650  CD1 LEU B  67      54.540  43.319  56.140  1.00 13.39           C
ANISOU 5650  CD1 LEU B  67     1732   1603   1751    -23    -51     -6       C
ATOM   5807  C   GLN B  78      47.225  38.787  55.119  1.00  8.92           C
ANISOU 5807  C   GLN B  78     1067   1219   1102    -10      8    -62       C
ATOM   5808  O   GLN B  78      48.410  38.488  55.143  1.00  8.25           O
ANISOU 5808  O   GLN B  78     1025   1038   1070     88    241   -162       O
ATOM   5809  N   TYR B  79      46.428  38.709  56.177  1.00  8.99           N
ANISOU 5809  N   TYR B  79     1002   1248   1165     74     55     -3       N
ATOM   5811  CA  TYR B  79      46.895  38.435  57.488  1.00  8.02           C
ANISOU 5811  CA  TYR B  79      839   1137   1070     54      1     -1       C
ATOM   5813  CB  TYR B  79      46.950  39.767  58.265  1.00  8.97           C
ANISOU 5813  CB  TYR B  79     1017   1308   1081     28    -40     50       C
ATOM   5816  CG  TYR B  79      47.829  40.783  57.637  1.00 10.67           C
ANISOU 5816  CG  TYR B  79     1470   1218   1366     33    -75    -29       C
ATOM   5817  CD1 TYR B  79      47.372  41.585  56.591  1.00 10.41           C
ANISOU 5817  CD1 TYR B  79     1287   1434   1233     48    -23     53       C
ATOM   5821  CZ  TYR B  79      49.508  42.647  56.456  1.00 11.42           C
ANISOU 5821  CZ  TYR B  79     1639   1375   1323     23   -103     73       C
ATOM   5824  CE2 TYR B  79      49.983  41.862  57.492  1.00 13.23           C
ANISOU 5824  CE2 TYR B  79     1691   1689   1643     97    -35    125       C
ATOM   5826  CD2 TYR B  79      49.149  40.954  58.078  1.00 10.33           C
ANISOU 5826  CD2 TYR B  79     1290   1228   1406    121    -37     68       C
ATOM   5828  C   TYR B  79      45.968  37.423  58.190  1.00  9.02           C
ANISOU 5828  C   TYR B  79      968   1329   1128     34     -5     41       C
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ATOM   5829  O   TYR B  79      44.711  37.440  57.977  1.00  9.52           O
ANISOU 5829  O   TYR B  79      773   1538   1304     14     55     65       O
ATOM   5830  N   ALA B  80      46.571  36.536  58.984  1.00  7.80           N
ANISOU 5830  N   ALA B  80      819   1031   1112    115     44     12       N
ATOM   5832  CA  ALA B  80      45.854  35.619  59.849  1.00  8.40           C
ANISOU 5832  CA  ALA B  80      998   1151   1041     66     -4      9       C
ATOM   5834  CB  ALA B  80      45.566  34.241  59.164  1.00  7.99           C
ANISOU 5834  CB  ALA B  80      828   1188   1018     -9     -9     35       C
ATOM   5838  C   ALA B  80      46.657  35.400  61.149  1.00  9.34           C
ANISOU 5838  C   ALA B  80     1149   1279   1120     16    -36     49       C
ATOM   5839  O   ALA B  80      47.867  35.540  61.200  1.00  8.68           O
ANISOU 5839  O   ALA B  80     1091   1323    884    239   -125    131       O
ATOM   5840  N   VAL B  81      45.926  35.078  62.194  1.00  9.78           N
ANISOU 5840  N   VAL B  81     1170   1395   1151     56      3     33       N
ATOM   5842  CA  VAL B  81      46.490  34.876  63.510  1.00 10.70           C
ANISOU 5842  CA  VAL B  81     1382   1466   1217     -1     -3    -18       C
ATOM   5844  CB  VAL B  81      45.440  35.381  64.540  1.00 10.77           C
ANISOU 5844  CB  VAL B  81     1355   1459   1275     73   -125    -40       C
ATOM   5846  CG1 VAL B  81      45.844  34.991  65.963  1.00 15.07           C
ANISOU 5846  CG1 VAL B  81     2122   2004   1596    -12      8     10       C
ATOM   5850  CG2 VAL B  81      45.255  36.854  64.391  1.00 11.08           C
ANISOU 5850  CG2 VAL B  81     1359   1557   1291     -7     -5   -129       C
ATOM   5854  C   VAL B  81      46.766  33.405  63.798  1.00 10.54           C
ANISOU 5854  C   VAL B  81     1348   1426   1231    -36     17     -5       C
ATOM   5855  O   VAL B  81      45.964  32.542  63.439  1.00 10.69           O
ANISOU 5855  O   VAL B  81     1345   1493   1224   -170   -151    -83       O
ATOM   5856  N   GLN B  82      47.911  33.116  64.414  1.00 10.66           N
ANISOU 5856  N   GLN B  82     1423   1342   1284   -102     25     22       N
ATOM   5858  CA  GLN B  82      48.188  31.819  65.022  1.00 10.04           C
ANISOU 5858  CA  GLN B  82     1313   1268   1234     13     -5     38       C
ATOM   5860  CB  GLN B  82      49.594  31.337  64.689  1.00  9.48           C
ANISOU 5860  CB  GLN B  82     1232   1262   1107    -46    127     70       C
ATOM   5863  CG  GLN B  82      49.974  30.000  65.256  1.00  7.09           C
ANISOU 5863  CG  GLN B  82     1047   1081    563    -69    230     -8       C
ATOM   5866  CD  GLN B  82      51.323  29.560  64.910  1.00  8.66           C
ANISOU 5866  CD  GLN B  82     1307   1041    939     -4     29    123       C
ATOM   5867  OE1 GLN B  82      52.258  30.389  64.823  1.00 10.82           O
ANISOU 5867  OE1 GLN B  82     1045   1502   1562    156    105    -69       O
ATOM   5868  NE2 GLN B  82      51.485  28.221  64.712  1.00 11.05           N
ANISOU 5868  NE2 GLN B  82     1410   1351   1437     57    110   -109       N
ATOM   5871  C   GLN B  82      48.008  32.004  66.552  1.00 10.14           C
ANISOU 5871  C   GLN B  82     1375   1204   1270     19    -74     21       C
ATOM   5872  O   GLN B  82      48.691  32.824  67.151  1.00  8.93           O
ANISOU 5872  O   GLN B  82     930   1355   1106     13   -342    210       O
ATOM   5873  N   PRO B  83      47.032  31.342  67.180  1.00 11.13           N
ANISOU 5873  N   PRO B  83     1383   1422   1424     65    -79      9       N
ATOM   5874  CA  PRO B  83      46.794  31.558  68.615  1.00 12.40           C
ANISOU 5874  CA  PRO B  83     1564   1595   1549      5     -2     53       C
ATOM   5876  CB  PRO B  83      45.618  30.622  68.920  1.00 12.26           C
ANISOU 5876  CB  PRO B  83     1470   1634   1555      0     -4     12       C
ATOM   5879  CG  PRO B  83      44.973  30.361  67.633  1.00 12.89           C
ANISOU 5879  CG  PRO B  83     1616   1658   1623     84    -42     14       C
ATOM   5882  CD  PRO B  83      45.992  30.469  66.589  1.00 11.71           C
ANISOU 5882  CD  PRO B  83     1617   1235   1594     -4     18     67       C
ATOM   5885  C   PRO B  83      47.988  31.235  69.504  1.00 12.77           C
ANISOU 5885  C   PRO B  83     1594   1684   1572     -2      8     26       C
ATOM   5886  O   PRO B  83      48.290  31.988  70.456  1.00 13.42           O
ANISOU 5886  O   PRO B  83     1641   1795   1663     10    117    -64       O
ATOM   5887  N   SER B  84      48.688  30.162  69.172  1.00 12.21           N
ANISOU 5887  N   SER B  84     1531   1614   1495      3     26     28       N
ATOM   5889  CA  SER B  84      49.863  29.755  69.930  1.00 12.54           C
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ANISOU 5889  CA  SER B  84     1536   1619   1608     81    -27     15       C
ATOM   5891  CB  SER B  84      49.444  28.734  70.964  1.00 12.66           C
ANISOU 5891  CB  SER B  84     1490   1737   1582     44     12     14       C
ATOM   5894  OG  SER B  84      50.498  28.512  71.895  1.00 18.45           O
ANISOU 5894  OG  SER B  84     2286   2435   2286    184   -178    177       O
ATOM   5896  C   SER B  84      50.889  29.158  68.970  1.00 11.40           C
ANISOU 5896  C   SER B  84     1325   1552   1452     -4     30     33       C
ATOM   5897  O   SER B  84      50.519  28.540  68.005  1.00  9.30           O
ANISOU 5897  O   SER B  84      640   1614   1277    283    -63    121       O
ATOM   5898  N   PRO B  85      52.177  29.291  69.256  1.00 12.42           N
ANISOU 5898  N   PRO B  85     1526   1648   1544     97   -156    -57       N
ATOM   5899  CA  PRO B  85      53.217  28.842  68.342  1.00 12.47           C
ANISOU 5899  CA  PRO B  85     1467   1686   1582     43   -119     22       C
ATOM   5901  CB  PRO B  85      54.462  29.635  68.802  1.00 13.15           C
ANISOU 5901  CB  PRO B  85     1596   1680   1720    110   -152    -22       C
ATOM   5904  CG  PRO B  85      54.231  29.887  70.211  1.00 14.30           C
ANISOU 5904  CG  PRO B  85     1671   1984   1777      0    -14     17       C
ATOM   5907  CD  PRO B  85      52.730  29.931  70.461  1.00 13.75           C
ANISOU 5907  CD  PRO B  85     1689   1882   1653     90   -149    -11       C
ATOM   5910  C   PRO B  85      53.397  27.317  68.465  1.00 12.17           C
ANISOU 5910  C   PRO B  85     1455   1641   1525     78    -53    -40       C
ATOM   5911  O   PRO B  85      54.399  26.805  68.968  1.00 12.15           O
ANISOU 5911  O   PRO B  85     1560   1608   1447    248   -205     -8       O
ATOM   5912  N   ASP B  86      52.403  26.612  67.976  1.00 10.80           N
ANISOU 5912  N   ASP B  86     1346   1566   1190     71     73    -58       N
ATOM   5914  CA  ASP B  86      52.321  25.228  68.124  1.00 11.92           C
ANISOU 5914  CA  ASP B  86     1467   1571   1489     91     28    -10       C
ATOM   5916  CB  ASP B  86      50.908  24.816  68.556  1.00 13.23           C
ANISOU 5916  CB  ASP B  86     1610   1710   1707     14     21     -1       C
ATOM   5919  CG  ASP B  86      50.524  25.368  69.911  1.00 16.05           C
ANISOU 5919  CG  ASP B  86     1988   2059   2050    117     11    -27       C
ATOM   5920  OD1 ASP B  86      51.380  25.878  70.662  1.00 18.77           O
ANISOU 5920  OD1 ASP B  86     2721   2285   2124     10   -163   -105       O
ATOM   5921  OD2 ASP B  86      49.347  25.373  70.284  1.00 20.09           O
ANISOU 5921  OD2 ASP B  86     2402   2714   2517   -259    571     94       O
ATOM   5922  C   ASP B  86      52.749  24.456  66.903  1.00 10.99           C
ANISOU 5922  C   ASP B  86     1304   1560   1311    -24    -41      4       C
ATOM   5923  O   ASP B  86      52.488  23.239  66.792  1.00 10.78           O
ANISOU 5923  O   ASP B  86     1135   1522   1437    107     27     18       O
ATOM   5924  N   GLY B  87      53.509  25.127  66.039  1.00 10.42           N
ANISOU 5924  N   GLY B  87     1385   1337   1237    -49    -58    -38       N
ATOM   5926  CA  GLY B  87      54.169  24.415  64.992  1.00 10.02           C
ANISOU 5926  CA  GLY B  87     1194   1298   1314     19     34    -33       C
ATOM   5929  C   GLY B  87      54.118  25.023  63.635  1.00  9.38           C
ANISOU 5929  C   GLY B  87     1162   1219   1180     20    -32    -52       C
ATOM   5930  O   GLY B  87      53.076  25.566  63.254  1.00  9.96           O
ANISOU 5930  O   GLY B  87     1142   1342   1298     58    -10   -221       O
ATOM   5931  N   LEU B  88      55.211  24.879  62.865  1.00  8.48           N
ANISOU 5931  N   LEU B  88      822   1253   1145     80    -33    -16       N
ATOM   5933  CA  LEU B  88      55.203  25.427  61.519  1.00  8.82           C
ANISOU 5933  CA  LEU B  88     1060   1136   1154      7     23     14       C
ATOM   5935  CB  LEU B  88      56.572  25.229  60.799  1.00 10.10           C
ANISOU 5935  CB  LEU B  88     1193   1479   1165    247    -69    117       C
ATOM   5938  CG  LEU B  88      57.905  25.603  61.452  1.00 14.21           C
ANISOU 5938  CG  LEU B  88     1630   1663   2104   -107    144   -172       C
ATOM   5940  CD1 LEU B  88      58.993  25.661  60.326  1.00 14.60           C
ANISOU 5940  CD1 LEU B  88     2193   1639   1711    -54    212    -33       C
ATOM   5944  CD2 LEU B  88      58.016  26.696  62.462  1.00 14.11           C
ANISOU 5944  CD2 LEU B  88     1655   2028   1677   -186    141    -42       C
ATOM   5948  C   LEU B  88      54.082  24.864  60.625  1.00  9.53           C
ANISOU 5948  C   LEU B  88     1173   1222   1222     69    -14     23       C
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ATOM   5949  O   LEU B  88      53.530  25.574  59.786  1.00 10.11           O
ANISOU 5949  O   LEU B  88    1371   1282   1185    -31   -118     18       O
ATOM   5950  N   ALA B  89      53.706  23.606  60.819  1.00  8.94           N
ANISOU 5950  N   ALA B  89    1045   1132   1218     91   -150      0       N
ATOM   5952  CA  ALA B  89      52.765  22.981  59.902  1.00  9.57           C
ANISOU 5952  CA  ALA B  89    1212   1224   1199     55     -3     -3       C
ATOM   5954  CB  ALA B  89      52.767  21.503  60.034  1.00  9.73           C
ANISOU 5954  CB  ALA B  89    1068   1316   1311    -83    -19    -25       C
ATOM   5958  C   ALA B  89      51.392  23.579  60.120  1.00  9.00           C
ANISOU 5958  C   ALA B  89    1043   1138   1238     33    -31    -16       C
ATOM   5959  O   ALA B  89      50.498  23.454  59.288  1.00 10.03           O
ANISOU 5959  O   ALA B  89    1489   1303   1019    208     -1   -102       O
ATOM   5960  N   GLN B  90      51.207  24.247  61.247  1.00  9.06           N
ANISOU 5960  N   GLN B  90    1012   1281   1149     -7    -53     35       N
ATOM   5962  CA  GLN B  90      49.923  24.907  61.453  1.00  9.73           C
ANISOU 5962  CA  GLN B  90    1261   1141   1291     50     13     18       C
ATOM   5964  CB  GLN B  90      49.785  25.542  62.825  1.00 10.40           C
ANISOU 5964  CB  GLN B  90    1271   1419   1261    -57     -7     69       C
ATOM   5967  CG  GLN B  90      49.780  24.593  63.941  1.00 12.85           C
ANISOU 5967  CG  GLN B  90    1707   1528   1646    -59      0    117       C
ATOM   5970  CD  GLN B  90      49.222  25.221  65.212  1.00 13.58           C
ANISOU 5970  CD  GLN B  90    1782   1699   1678    105     71     62       C
ATOM   5971  OE1 GLN B  90      49.616  26.332  65.569  1.00 13.60           O
ANISOU 5971  OE1 GLN B  90    1934   1991   1242    183     25    -80       O
ATOM   5972  NE2 GLN B  90      48.358  24.486  65.923  1.00 12.42           N
ANISOU 5972  NE2 GLN B  90    1356   1676   1684     91    -38    -11       N
ATOM   5975  C   GLN B  90      49.691  25.990  60.395  1.00  9.64           C
ANISOU 5975  C   GLN B  90    1237   1207   1217     77     -7      6       C
ATOM   5976  O   GLN B  90      48.554  26.433  60.235  1.00  9.52           O
ANISOU 5976  O   GLN B  90    1004   1279   1332    230     32     10       O
ATOM   5977  N   ALA B  91      50.731  26.415  59.695  1.00  8.47           N
ANISOU 5977  N   ALA B  91     960    988   1268    125     62     36       N
ATOM   5979  CA  ALA B  91      50.552  27.450  58.664  1.00  9.50           C
ANISOU 5979  CA  ALA B  91    1061   1349   1199      2    132     73       C
ATOM   5981  CB  ALA B  91      51.960  27.870  58.032  1.00  8.79           C
ANISOU 5981  CB  ALA B  91     831   1234   1273    178     17    114       C
ATOM   5985  C   ALA B  91      49.587  26.956  57.593  1.00  9.35           C
ANISOU 5985  C   ALA B  91    1004   1353   1195     23    175     76       C
ATOM   5986  O   ALA B  91      48.787  27.723  57.021  1.00 10.16           O
ANISOU 5986  O   ALA B  91    1111   1516   1230     44     86    153       O
ATOM   5987  N   PHE B  92      49.601  25.666  57.334  1.00  9.52           N
ANISOU 5987  N   PHE B  92     906   1345   1363     23     99     67       N
ATOM   5989  CA  PHE B  92      48.744  25.151  56.274  1.00 10.66           C
ANISOU 5989  CA  PHE B  92    1235   1434   1381    -24     81     -2       C
ATOM   5991  CB  PHE B  92      49.331  23.909  55.685  1.00 10.52           C
ANISOU 5991  CB  PHE B  92    1237   1401   1358     22     -3     94       C
ATOM   5994  CG  PHE B  92      50.669  24.168  55.106  1.00 11.85           C
ANISOU 5994  CG  PHE B  92    1455   1571   1473    -91     16   -138       C
ATOM   5995  CD1 PHE B  92      51.792  24.028  55.880  1.00 12.75           C
ANISOU 5995  CD1 PHE B  92    1613   1740   1490    109   -116     75       C
ATOM   5997  CE1 PHE B  92      52.984  24.348  55.392  1.00 13.45           C
ANISOU 5997  CE1 PHE B  92    1713   1763   1633     91    -54   -182       C
ATOM   5999  CZ  PHE B  92      53.123  24.896  54.120  1.00 13.04           C
ANISOU 5999  CZ  PHE B  92    1657   1670   1627    158     90   -112       C
ATOM   6001  CE2 PHE B  92      52.030  25.087  53.363  1.00 12.75           C
ANISOU 6001  CE2 PHE B  92    1749   1517   1577     76     18    -27       C
ATOM   6003  CD2 PHE B  92      50.785  24.731  53.862  1.00 10.07           C
ANISOU 6003  CD2 PHE B  92    1330   1150   1346     36    -88     57       C
ATOM   6005  C   PHE B  92      47.274  24.951  56.715  1.00 10.32           C
ANISOU 6005  C   PHE B  92    1164   1372   1385      3     65      2       C
ATOM   6006  O   PHE B  92      46.420  24.797  55.876  1.00 11.89           O
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ANISOU 6006  O   PHE B  92     1268   1712   1536      4    262      9       O
ATOM   6007  N   LEU B  93      47.026  24.940  58.011  1.00 10.05           N
ANISOU 6007  N   LEU B  93     1256   1274   1289    -26     35    -23       N
ATOM   6009  CA  LEU B  93      45.694  24.731  58.538  1.00 11.00           C
ANISOU 6009  CA  LEU B  93     1382   1446   1351     62     55     19       C
ATOM   6011  CB  LEU B  93      45.726  23.953  59.873  1.00 11.63           C
ANISOU 6011  CB  LEU B  93     1442   1573   1402     55     48    -21       C
ATOM   6014  CG  LEU B  93      46.401  22.573  59.935  1.00 13.17           C
ANISOU 6014  CG  LEU B  93     1626   1645   1733    -20    -49     12       C
ATOM   6016  CD1 LEU B  93      46.303  21.974  61.335  1.00 15.24           C
ANISOU 6016  CD1 LEU B  93     1834   1938   2018      3     12    -42       C
ATOM   6020  CD2 LEU B  93      45.900  21.612  58.904  1.00 14.64           C
ANISOU 6020  CD2 LEU B  93     1689   1917   1956   -108    187    -64       C
ATOM   6024  C   LEU B  93      45.093  26.117  58.657  1.00 10.88           C
ANISOU 6024  C   LEU B  93     1371   1426   1335     -4     64     52       C
ATOM   6025  O   LEU B  93      43.991  26.376  58.160  1.00 10.87           O
ANISOU 6025  O   LEU B  93     1181   1628   1319    -63    264    207       O
ATOM   6026  N   ILE B  94      45.856  27.029  59.244  1.00 10.62           N
ANISOU 6026  N   ILE B  94     1310   1358   1366     68    110    -19       N
ATOM   6028  CA  ILE B  94      45.447  28.453  59.331  1.00  9.81           C
ANISOU 6028  CA  ILE B  94     1222   1231   1273     85    -50     21       C
ATOM   6030  CB  ILE B  94      46.467  29.249  60.086  1.00  9.86           C
ANISOU 6030  CB  ILE B  94     1230   1248   1267     42     34    -11       C
ATOM   6032  CG1 ILE B  94      46.521  28.794  61.545  1.00  9.26           C
ANISOU 6032  CG1 ILE B  94     1150   1108   1259     48     57      0       C
ATOM   6035  CD1 ILE B  94      47.680  29.341  62.241  1.00 10.93           C
ANISOU 6035  CD1 ILE B  94     1540   1389   1223     63   -167     58       C
ATOM   6039  CG2 ILE B  94      46.192  30.752  60.003  1.00 10.67           C
ANISOU 6039  CG2 ILE B  94     1310   1358   1385     28   -244     36       C
ATOM   6043  C   ILE B  94      45.230  29.044  57.942  1.00  8.96           C
ANISOU 6043  C   ILE B  94     1128   1150   1125     77     -7    -53       C
ATOM   6044  O   ILE B  94      44.209  29.739  57.708  1.00  7.40           O
ANISOU 6044  O   ILE B  94     720   1160    929    220    -68   -225       O
ATOM   6045  N   GLY B  95      46.110  28.688  57.029  1.00  8.38           N
ANISOU 6045  N   GLY B  95     931   1124   1128     59   -104    -34       N
ATOM   6047  CA  GLY B  95      46.096  29.181  55.671  1.00  8.42           C
ANISOU 6047  CA  GLY B  95     1022   1014   1163     46     32     -5       C
ATOM   6050  C   GLY B  95      45.349  28.347  54.643  1.00  8.32           C
ANISOU 6050  C   GLY B  95     956   1039   1164     98     13    -31       C
ATOM   6051  O   GLY B  95      45.515  28.594  53.469  1.00  7.83           O
ANISOU 6051  O   GLY B  95     888   1020   1068    155   -152    -35       O
ATOM   6052  N   GLU B  96      44.507  27.396  55.076  1.00  9.91           N
ANISOU 6052  N   GLU B  96     1306   1180   1280    131     56     64       N
ATOM   6092  CE2 PHE B  98      48.406  32.421  50.809  1.00  8.04           C
ANISOU 6092  CE2 PHE B  98     873   1038   1141    -16    134    -53       C
ATOM   6094  CD2 PHE B  98      47.329  31.833  51.489  1.00  7.22           C
ANISOU 6094  CD2 PHE B  98     870   1059    813    -80   -116   -110       C
ATOM   6107  CD1 ILE B  99      48.292  26.722  52.011  1.00 10.09           C
ANISOU 6107  CD1 ILE B  99     1492   1202   1140    144     26   -113       C
ATOM   6180  N   ALA B 105      54.005  28.271  49.038  1.00  9.13           N
ANISOU 6180  N   ALA B 105     1049   1238   1181     70   -117   -132       N
ATOM   6182  CA  ALA B 105      55.381  28.388  49.531  1.00  9.04           C
ANISOU 6182  CA  ALA B 105     1060   1191   1183     18    -33    -63       C
ATOM   6184  CB  ALA B 105      56.253  29.230  48.596  1.00  8.45           C
ANISOU 6184  CB  ALA B 105     815   1231   1164    168    129   -103       C
ATOM   6188  C   ALA B 105      55.306  28.999  50.919  1.00  9.68           C
ANISOU 6188  C   ALA B 105     1123   1268   1285     99    -75    -94       C
ATOM   6189  O   ALA B 105      54.538  29.894  51.166  1.00 10.56           O
ANISOU 6189  O   ALA B 105     1437   1187   1385    419   -205   -179       O
ATOM   6190  N   LEU B 106      56.079  28.436  51.826  1.00  8.73           N
ANISOU 6190  N   LEU B 106     1185   1077   1054     77    -77     92       N
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ATOM   6192  CA  LEU B 106      56.207  28.942  53.154  1.00  8.22           C
ANISOU 6192  CA  LEU B 106      999   1054   1069     42     15     15       C
ATOM   6194  CB  LEU B 106      55.882  27.798  54.109  1.00  8.63           C
ANISOU 6194  CB  LEU B 106      911   1341   1024   -121    -96     57       C
ATOM   6197  CG  LEU B 106      56.131  28.037  55.595  1.00  9.16           C
ANISOU 6197  CG  LEU B 106     1132   1223   1123   -100     23    -57       C
ATOM   6199  CD1 LEU B 106      55.385  29.180  56.142  1.00  8.85           C
ANISOU 6199  CD1 LEU B 106      553   1515   1292    118    142    157       C
ATOM   6203  CD2 LEU B 106      55.825  26.772  56.362  1.00  8.50           C
ANISOU 6203  CD2 LEU B 106     1056   1061   1110     90   -105    -32       C
ATOM   6207  C   LEU B 106      57.656  29.392  53.380  1.00  8.53           C
ANISOU 6207  C   LEU B 106     1094   1156    990     53     -5      8       C
ATOM   6208  O   LEU B 106      58.637  28.618  53.077  1.00 10.31           O
ANISOU 6208  O   LEU B 106     1389   1380   1146    200    -29    -35       O
ATOM   6209  N   VAL B 107      57.815  30.606  53.914  1.00  9.20           N
ANISOU 6209  N   VAL B 107      994   1227   1274     71     86    111       N
ATOM   6211  CA  VAL B 107      59.086  31.091  54.369  1.00  8.45           C
ANISOU 6211  CA  VAL B 107     1127   1016   1068     -5     -5    -44       C
ATOM   6213  CB  VAL B 107      59.669  32.219  53.447  1.00  8.09           C
ANISOU 6213  CB  VAL B 107      994   1167    913      3     66     14       C
ATOM   6215  CG1 VAL B 107      58.815  33.497  53.546  1.00  8.02           C
ANISOU 6215  CG1 VAL B 107     1117    933    994   -102     17    -30       C
ATOM   6219  CG2 VAL B 107      61.097  32.542  53.818  1.00 11.35           C
ANISOU 6219  CG2 VAL B 107     1411   1295   1603     92    -92    -64       C
ATOM   6223  C   VAL B 107      58.941  31.543  55.837  1.00  8.32           C
ANISOU 6223  C   VAL B 107     1038   1136    985     32    136     43       C
ATOM   6224  O   VAL B 107      57.908  32.086  56.284  1.00  7.58           O
ANISOU 6224  O   VAL B 107      883   1211    784     90    235   -140       O
ATOM   6225  N   LEU B 108      59.970  31.232  56.591  1.00  7.68           N
ANISOU 6225  N   LEU B 108      857   1075    983     70     85     33       N
ATOM   6227  CA  LEU B 108      60.051  31.596  58.009  1.00  8.53           C
ANISOU 6227  CA  LEU B 108     1135   1010   1094     15     -7     21       C
ATOM   6229  CB  LEU B 108      61.048  30.678  58.695  1.00  8.58           C
ANISOU 6229  CB  LEU B 108     1056   1185   1015     -6      2     86       C
ATOM   6232  CG  LEU B 108      60.618  29.207  58.633  1.00  8.97           C
ANISOU 6232  CG  LEU B 108     1156   1113   1139    137     20    -64       C
ATOM   6234  CD1 LEU B 108      61.423  28.389  59.594  1.00 10.92           C
ANISOU 6234  CD1 LEU B 108     1506   1291   1350    -97    -25    223       C
ATOM   6238  CD2 LEU B 108      59.183  28.999  58.920  1.00 13.97           C
ANISOU 6238  CD2 LEU B 108     1668   1709   1927     91     44     20       C
ATOM   6242  C   LEU B 108      60.467  33.038  58.193  1.00  9.21           C
ANISOU 6242  C   LEU B 108     1198   1096   1204    -18      9     37       C
ATOM   6243  O   LEU B 108      61.370  33.529  57.533  1.00  9.90           O
ANISOU 6243  O   LEU B 108     1292   1117   1350    -99     78     -6       O
ATOM   6244  N   GLY B 109      59.805  33.700  59.120  1.00  9.66           N
ANISOU 6244  N   GLY B 109     1258   1163   1247   -154    115     67       N
ATOM   6246  CA  GLY B 109      60.014  35.112  59.347  1.00 10.34           C
ANISOU 6246  CA  GLY B 109     1424   1195   1308    -48     76    -92       C
ATOM   6249  C   GLY B 109      61.409  35.594  59.786  1.00 10.72           C
ANISOU 6249  C   GLY B 109     1319   1301   1451    -33     84     35       C
ATOM   6250  O   GLY B 109      61.710  36.784  59.600  1.00 13.56           O
ANISOU 6250  O   GLY B 109     1777   1530   1845   -170     -1    117       O
ATOM   6251  N   ASP B 110      62.202  34.762  60.441  1.00  9.78           N
ANISOU 6251  N   ASP B 110     1274   1173   1266    -53     68     34       N
ATOM   6253  CA  ASP B 110      63.532  35.128  60.905  1.00  9.40           C
ANISOU 6253  CA  ASP B 110     1233   1091   1247    -58     95    -20       C
ATOM   6255  CB  ASP B 110      63.814  34.749  62.362  1.00  9.23           C
ANISOU 6255  CB  ASP B 110     1075   1074   1356    -71    -21     56       C
ATOM   6258  CG  ASP B 110      63.702  33.203  62.666  1.00 12.59           C
ANISOU 6258  CG  ASP B 110     1778   1345   1659   -117    -82     89       C
ATOM   6259  OD1 ASP B 110      63.453  32.382  61.753  1.00 14.33           O
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ANISOU 6259  OD1 ASP B 110     2035   1474   1934    117    172    118       O
ATOM   6260  OD2 ASP B 110      63.825  32.741  63.839  1.00 15.01           O
ANISOU 6260  OD2 ASP B 110     2374   1602   1726   -207    -54     59       O
ATOM   6261  C   ASP B 110      64.597  34.525  60.028  1.00 10.65           C
ANISOU 6261  C   ASP B 110     1379   1253   1415     53     -9     21       C
ATOM   6262  O   ASP B 110      65.683  34.434  60.466  1.00 11.23           O
ANISOU 6262  O   ASP B 110     1206   1486   1576    -27     71   -122       O
ATOM   6263  N   ASN B 111      64.262  34.072  58.820  1.00  9.85           N
ANISOU 6263  N   ASN B 111     1376   1111   1254    -57      9    -39       N
ATOM   6265  CA  ASN B 111      65.297  33.533  57.911  1.00  9.92           C
ANISOU 6265  CA  ASN B 111     1204   1250   1312     25    -29     36       C
ATOM   6267  CB  ASN B 111      64.813  32.270  57.170  1.00 10.67           C
ANISOU 6267  CB  ASN B 111     1299   1417   1336    -10    -72    -53       C
ATOM   6270  CG  ASN B 111      64.890  30.962  57.979  1.00 11.50           C
ANISOU 6270  CG  ASN B 111     1509   1450   1410     77    -37     -9       C
ATOM   6271  OD1 ASN B 111      65.146  29.946  57.368  1.00 11.48           O
ANISOU 6271  OD1 ASN B 111     1002   1601   1757     97    -33   -236       O
ATOM   6272  ND2 ASN B 111      64.595  30.956  59.302  1.00  9.14           N
ANISOU 6272  ND2 ASN B 111      729   1293   1450    238    201   -153       N
ATOM   6275  C   ASN B 111      65.711  34.553  56.868  1.00 10.47           C
ANISOU 6275  C   ASN B 111     1218   1426   1332      6     79     14       C
ATOM   6276  O   ASN B 111      64.878  35.123  56.158  1.00 11.11           O
ANISOU 6276  O   ASN B 111     1014   1732   1475     93    345     93       O
ATOM   6277  N   LEU B 112      67.018  34.729  56.725  1.00  8.72           N
ANISOU 6277  N   LEU B 112      957   1229   1127    103      8      5       N
ATOM   6279  CA  LEU B 112      67.577  35.716  55.835  1.00 10.72           C
ANISOU 6279  CA  LEU B 112     1322   1374   1377     58     35    -22       C
ATOM   6281  CB  LEU B 112      68.444  36.698  56.657  1.00 10.59           C
ANISOU 6281  CB  LEU B 112     1213   1348   1460     62    -92    -33       C
ATOM   6284  CG  LEU B 112      68.836  37.998  55.916  1.00 15.52           C
ANISOU 6284  CG  LEU B 112     2092   1879   1925    -24    -53     -7       C
ATOM   6286  CD1 LEU B 112      69.423  39.166  56.816  1.00 16.60           C
ANISOU 6286  CD1 LEU B 112     2240   1995   2071    -51   -172    -15       C
ATOM   6290  CD2 LEU B 112      69.775  37.779  54.873  1.00 17.98           C
ANISOU 6290  CD2 LEU B 112     2259   2301   2271     -1     76   -163       C
ATOM   6294  C   LEU B 112      68.475  34.973  54.827  1.00  9.88           C
ANISOU 6294  C   LEU B 112     1175   1368   1209     75     80      2       C
ATOM   6295  O   LEU B 112      69.411  34.350  55.217  1.00 11.66           O
ANISOU 6295  O   LEU B 112     1490   1423   1514    112     11     82       O
ATOM   6296  N   TYR B 113      68.162  35.030  53.563  1.00  9.61           N
ANISOU 6296  N   TYR B 113     1127   1258   1266     59     42     -9       N
ATOM   6298  CA  TYR B 113      68.953  34.395  52.503  1.00  7.80           C
ANISOU 6298  CA  TYR B 113      999   1040    923      4     94     26       C
ATOM   6300  CB  TYR B 113      68.065  33.564  51.581  1.00  7.86           C
ANISOU 6300  CB  TYR B 113     1027   1071    886      7    152     26       C
ATOM   6303  CG  TYR B 113      67.339  32.444  52.224  1.00  9.60           C
ANISOU 6303  CG  TYR B 113     1325   1269   1053    -43    -63     29       C
ATOM   6304  CD1 TYR B 113      66.069  32.627  52.749  1.00 11.51           C
ANISOU 6304  CD1 TYR B 113     1341   1555   1476     -4     99     21       C
ATOM   6306  CE1 TYR B 113      65.378  31.548  53.357  1.00 10.21           C
ANISOU 6306  CE1 TYR B 113     1180   1285   1413     23     46      8       C
ATOM   6308  CZ  TYR B 113      65.973  30.311  53.427  1.00 11.84           C
ANISOU 6308  CZ  TYR B 113     1573   1440   1484     -3     84     54       C
ATOM   6309  OH  TYR B 113      65.307  29.256  54.015  1.00 10.12           O
ANISOU 6309  OH  TYR B 113      946   1215   1681    158   -103    326       O
ATOM   6311  CE2 TYR B 113      67.183  30.109  52.837  1.00 11.43           C
ANISOU 6311  CE2 TYR B 113     1157   1317   1868     72   -151    158       C
ATOM   6313  CD2 TYR B 113      67.860  31.177  52.211  1.00 10.78           C
ANISOU 6313  CD2 TYR B 113     1431   1394   1271    115   -249    126       C
ATOM   6315  C   TYR B 113      69.639  35.484  51.642  1.00  7.73           C
ANISOU 6315  C   TYR B 113     1030   1027    878     43     56     33       C
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ATOM   6316  O   TYR B 113      69.122  36.576  51.488  1.00  7.43           O
ANISOU 6316  O   TYR B 113    1163   1019    639     56    111    197        O
ATOM   6317  N   TYR B 114      70.843  35.209  51.135  1.00  7.30           N
ANISOU 6317  N   TYR B 114    1038    916    817     78     37    -24        N
ATOM   6319  CA  TYR B 114      71.408  36.134  50.234  1.00  7.79           C
ANISOU 6319  CA  TYR B 114     882   1085    990     69     20     22        C
ATOM   6321  CB  TYR B 114      72.075  37.313  50.967  1.00  8.84           C
ANISOU 6321  CB  TYR B 114    1069   1172   1115     76     64     44        C
ATOM   6383  CD1 PHE B 118      68.327  32.317  47.151  1.00 11.71           C
ANISOU 6383  CD1 PHE B 118    1659   1400   1388     23    178     61        C
ATOM   6385  CE1 PHE B 118      67.478  31.934  48.165  1.00 10.86           C
ANISOU 6385  CE1 PHE B 118    1297   1145   1683   -313    161   -107        C
ATOM   6387  CZ  PHE B 118      66.568  32.812  48.671  1.00 11.10           C
ANISOU 6387  CZ  PHE B 118    1255   1529   1430    -14    159    112        C
ATOM   6389  CE2 PHE B 118      66.565  34.096  48.281  1.00  8.70           C
ANISOU 6389  CE2 PHE B 118     957   1364    982     81     60   -100        C
ATOM   6391  CD2 PHE B 118      67.419  34.500  47.291  1.00 10.35           C
ANISOU 6391  CD2 PHE B 118     951   1393   1588   -123    128    124        C
ATOM   6441  CD2 LEU B 121      68.933  28.316  46.002  1.00 14.06           C
ANISOU 6441  CD2 LEU B 121    1921   1916   1505      9    196     85        C
ATOM   6460  CD2 LEU B 122      63.707  31.467  46.720  1.00  9.31           C
ANISOU 6460  CD2 LEU B 122    1313   1116   1108   -102     70    113        C
ATOM   6586  CA  ALA B 132      57.759  19.555  47.596  1.00  7.62           C
ANISOU 6586  CA  ALA B 132    1079    829    987     20      6    -63        C
ATOM   6588  CB  ALA B 132      57.651  19.081  48.995  1.00  7.68           C
ANISOU 6588  CB  ALA B 132     999    839   1077    -14   -149    -79        C
ATOM   6592  C   ALA B 132      59.193  19.811  47.242  1.00  7.81           C
ANISOU 6592  C   ALA B 132    1048    937    982     -1   -135    -92        C
ATOM   6593  O   ALA B 132      59.901  18.907  46.753  1.00  9.52           O
ANISOU 6593  O   ALA B 132    1201   1199   1213    -23    -45   -180        O
ATOM   6594  N   SER B 133      59.624  21.054  47.457  1.00  7.96           N
ANISOU 6594  N   SER B 133    1120    955    946      4     24     57        N
ATOM   6596  CA  SER B 133      61.003  21.436  47.325  1.00  7.43           C
ANISOU 6596  CA  SER B 133     863   1003    957     13    -60    -44        C
ATOM   6598  CB  SER B 133      61.254  22.334  46.130  1.00  7.20           C
ANISOU 6598  CB  SER B 133     722    952   1061      9    -42     -6        C
ATOM   6603  C   SER B 133      61.483  22.145  48.596  1.00  7.62           C
ANISOU 6603  C   SER B 133     986    957    950     14     48    -40        C
ATOM   6604  O   SER B 133      60.831  23.068  49.081  1.00  8.09           O
ANISOU 6604  O   SER B 133     941   1173    958    -58    192   -139        O
ATOM   6605  N   VAL B 134      62.653  21.739  49.068  1.00  6.84           N
ANISOU 6605  N   VAL B 134     804    875    916     48    102   -104        N
ATOM   6607  CA  VAL B 134      63.297  22.261  50.256  1.00  6.93           C
ANISOU 6607  CA  VAL B 134     868    930    834     19     -8    -46        C
ATOM   6609  CB  VAL B 134      63.078  21.349  51.462  1.00  8.11           C
ANISOU 6609  CB  VAL B 134    1060   1036    985    -19     65    -54        C
ATOM   6611  CG1 VAL B 134      61.631  21.151  51.670  1.00  8.90           C
ANISOU 6611  CG1 VAL B 134    1228   1338    814    -69    -51     20        C
ATOM   6615  CG2 VAL B 134      63.850  20.005  51.357  1.00  9.68           C
ANISOU 6615  CG2 VAL B 134    1360   1156   1158   -123     20     12        C
ATOM   6619  C   VAL B 134      64.797  22.369  49.946  1.00  7.97           C
ANISOU 6619  C   VAL B 134     995   1003   1027    -43      0    -43        C
ATOM   6620  O   VAL B 134      65.247  21.827  48.978  1.00  9.70           O
ANISOU 6620  O   VAL B 134    1066   1341   1278    -36   -109   -156        O
ATOM   6621  N   PHE B 135      65.546  23.086  50.772  1.00  7.57           N
ANISOU 6621  N   PHE B 135    1017   1087    770     15    -49    -23        N
ATOM   6623  CA  PHE B 135      66.943  23.426  50.530  1.00  8.09           C
ANISOU 6623  CA  PHE B 135    1012   1097    963     73    -29      1        C
ATOM   6625  CB  PHE B 135      67.060  24.916  50.305  1.00  8.70           C
ANISOU 6625  CB  PHE B 135     832   1327   1146    -61     51     -8        C
ATOM   6628  CG  PHE B 135      66.273  25.377  49.135  1.00 10.94           C
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ANISOU 6628  CG  PHE B 135     1378   1321   1455    -61    -99    -36       C
ATOM   6629  CD1 PHE B 135      64.942  25.787  49.294  1.00 14.22           C
ANISOU 6629  CD1 PHE B 135     1604   1903   1893     17      3    -14       C
ATOM   6631  CE1 PHE B 135      64.203  26.127  48.196  1.00 16.39           C
ANISOU 6631  CE1 PHE B 135     1777   2233   2218    141     77     76       C
ATOM   6633  CZ  PHE B 135      64.778  26.094  46.936  1.00 17.11           C
ANISOU 6633  CZ  PHE B 135     2309   2123   2068     20   -158     43       C
ATOM   6635  CE2 PHE B 135      66.033  25.682  46.784  1.00 15.86           C
ANISOU 6635  CE2 PHE B 135     2082   2010   1932    -51     76     89       C
ATOM   6637  CD2 PHE B 135      66.787  25.306  47.883  1.00 14.39           C
ANISOU 6637  CD2 PHE B 135     1818   1885   1763    -16     78     51       C
ATOM   6639  C   PHE B 135      67.798  22.981  51.711  1.00  8.70           C
ANISOU 6639  C   PHE B 135     1170   1129   1004     46    -36    -35       C
ATOM   6640  O   PHE B 135      67.394  23.171  52.873  1.00  9.72           O
ANISOU 6640  O   PHE B 135     1520   1230    940    -29    -39    247       O
ATOM   6641  N   ALA B 136      68.910  22.321  51.386  1.00  7.74           N
ANISOU 6641  N   ALA B 136      892   1086    961    -16    -61    100       N
ATOM   6643  CA  ALA B 136      69.870  21.847  52.388  1.00  7.69           C
ANISOU 6643  CA  ALA B 136      965    998    958     -3    -41     84       C
ATOM   6645  CB  ALA B 136      70.215  20.419  52.076  1.00  8.30           C
ANISOU 6645  CB  ALA B 136      970   1226    956     17    -65     41       C
ATOM   6649  C   ALA B 136      71.120  22.726  52.405  1.00  8.69           C
ANISOU 6649  C   ALA B 136     1163   1108   1030     -9     -2     55       C
ATOM   6650  O   ALA B 136      71.699  23.024  51.348  1.00  9.88           O
ANISOU 6650  O   ALA B 136     1248   1395   1108   -236    212     50       O
ATOM   6651  N   TYR B 137      71.562  23.103  53.600  1.00  7.61           N
ANISOU 6651  N   TYR B 137     1117   1021    750    -86     47     79       N
ATOM   6653  CA  TYR B 137      72.668  24.023  53.761  1.00  7.01           C
ANISOU 6653  CA  TYR B 137      858    959    848     50    -29      4       C
ATOM   6655  CB  TYR B 137      72.170  25.396  54.039  1.00  5.60           C
ANISOU 6655  CB  TYR B 137      660    986    481    158     64    -15       C
ATOM   6658  CG  TYR B 137      73.094  26.593  54.050  1.00  7.74           C
ANISOU 6658  CG  TYR B 137      972    916   1050    145    -45     29       C
ATOM   6659  CD1 TYR B 137      73.395  27.309  52.887  1.00  8.47           C
ANISOU 6659  CD1 TYR B 137     1084   1200    931    -20    -28    -89       C
ATOM   6661  CE1 TYR B 137      74.172  28.474  52.929  1.00  8.41           C
ANISOU 6661  CE1 TYR B 137     1046   1076   1072    -32     10     87       C
ATOM   6663  CZ  TYR B 137      74.671  28.944  54.149  1.00  7.72           C
ANISOU 6663  CZ  TYR B 137      958    897   1076    -37     91     87       C
ATOM   6664  OH  TYR B 137      75.410  30.080  54.226  1.00  8.42           O
ANISOU 6664  OH  TYR B 137      896    941   1359   -155     38   -107       O
ATOM   6666  CE2 TYR B 137      74.379  28.295  55.304  1.00  5.35           C
ANISOU 6666  CE2 TYR B 137      523    792    718    208   -123    159       C
ATOM   6668  CD2 TYR B 137      73.603  27.079  55.236  1.00  9.47           C
ANISOU 6668  CD2 TYR B 137     1184   1225   1189     64     50   -110       C
ATOM   6670  C   TYR B 137      73.600  23.560  54.864  1.00  6.91           C
ANISOU 6670  C   TYR B 137      996    881    748     -6    -54     13       C
ATOM   6671  O   TYR B 137      73.138  23.215  55.943  1.00  6.59           O
ANISOU 6671  O   TYR B 137      916    777    810    -72    -25    -82       O
ATOM   6672  N   HIS B 138      74.892  23.489  54.518  1.00  5.78           N
ANISOU 6672  N   HIS B 138      761    682    750    -84      0     46       N
ATOM   6674  CA  HIS B 138      75.898  23.030  55.456  1.00  7.38           C
ANISOU 6674  CA  HIS B 138      962    860    980   -117      5     13       C
ATOM   6676  CB  HIS B 138      77.239  22.816  54.766  1.00  7.04           C
ANISOU 6676  CB  HIS B 138      882    754   1038    -86    -53    -59       C
ATOM   6679  CG  HIS B 138      78.208  22.038  55.560  1.00  7.62           C
ANISOU 6679  CG  HIS B 138     1045   1008    841    -85     77      5       C
ATOM   6680  ND1 HIS B 138      78.874  22.569  56.641  1.00  7.25           N
ANISOU 6680  ND1 HIS B 138      698   1154    899    -97   -265     16       N
ATOM   6682  CE1 HIS B 138      79.689  21.641  57.134  1.00 10.52           C
ANISOU 6682  CE1 HIS B 138     1577   1323   1097     46    -34    -95       C
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ATOM   6684  NE2 HIS B 138      79.591  20.553  56.399  1.00 10.01           N
ANISOU 6684  NE2 HIS B 138    1385    938   1480    -44     -5    188        N
ATOM   6686  CD2 HIS B 138      78.593  20.739  55.476  1.00 10.19           C
ANISOU 6686  CD2 HIS B 138    1297   1127   1448   -135    -63    -16        C
ATOM   6688  C   HIS B 138      76.043  24.035  56.579  1.00  8.16           C
ANISOU 6688  C   HIS B 138    1013    976   1110    -39    -35     -7        C
ATOM   6689  O   HIS B 138      76.275  25.202  56.340  1.00  7.93           O
ANISOU 6689  O   HIS B 138     956    838   1216   -142      0    -97        O
ATOM   6690  N   VAL B 139      75.977  23.554  57.798  1.00  8.34           N
ANISOU 6690  N   VAL B 139    1028   1039   1098   -196     33     20        N
ATOM   6692  CA  VAL B 139      76.073  24.411  58.971  1.00  9.44           C
ANISOU 6692  CA  VAL B 139    1208   1219   1160    -37     -4    -24        C
ATOM   6694  CB  VAL B 139      74.667  24.696  59.635  1.00  9.21           C
ANISOU 6694  CB  VAL B 139    1168   1183   1148    -35    -58      6        C
ATOM   6696  CG1 VAL B 139      73.811  25.510  58.743  1.00 11.13           C
ANISOU 6696  CG1 VAL B 139    1331   1479   1419     68     18     24        C
ATOM   6700  CG2 VAL B 139      73.947  23.396  60.109  1.00 11.01           C
ANISOU 6700  CG2 VAL B 139    1348   1453   1381    -95    -62    -29        C
ATOM   6704  C   VAL B 139      76.985  23.839  60.033  1.00  9.80           C
ANISOU 6704  C   VAL B 139    1299   1255   1168    -39    -23     -4        C
ATOM   6705  O   VAL B 139      77.306  22.617  60.057  1.00  9.37           O
ANISOU 6705  O   VAL B 139    1305   1253   1001      1   -149   -156        O
ATOM   6706  N   LEU B 140      77.391  24.727  60.951  1.00 10.87           N
ANISOU 6706  N   LEU B 140    1521   1324   1284    -31    -91    -36        N
ATOM   6708  CA  LEU B 140      78.219  24.302  62.084  1.00 12.83           C
ANISOU 6708  CA  LEU B 140    1660   1567   1646    -34   -118    -38        C
ATOM   6710  CB  LEU B 140      78.877  25.529  62.771  1.00 12.37           C
ANISOU 6710  CB  LEU B 140    1653   1531   1516    -59    -36    -81        C
ATOM   6713  CG  LEU B 140      79.758  25.214  63.970  1.00 14.74           C
ANISOU 6713  CG  LEU B 140    1823   1899   1878    -54    -73    -27        C
ATOM   6723  C   LEU B 140      77.442  23.534  63.146  1.00 12.95           C
ANISOU 6723  C   LEU B 140    1726   1589   1605    -97    -60    -64        C
ATOM   6724  O   LEU B 140      77.970  22.606  63.760  1.00 13.82           O
ANISOU 6724  O   LEU B 140    1831   1470   1950   -154    -75    -39        O
ATOM   6725  N   ASP B 141      76.194  23.896  63.387  1.00 13.93           N
ANISOU 6725  N   ASP B 141    1874   1734   1681    -43    -86    -59        N
ATOM   6727  CA  ASP B 141      75.470  23.282  64.525  1.00 15.67           C
ANISOU 6727  CA  ASP B 141    2062   1924   1967    -90      2    -33        C
ATOM   6729  CB  ASP B 141      75.302  24.274  65.696  1.00 17.30           C
ANISOU 6729  CB  ASP B 141    2319   2077   2178    -72    124    -46        C
ATOM   6732  CG  ASP B 141      76.599  24.454  66.503  1.00 24.35           C
ANISOU 6732  CG  ASP B 141    3033   3149   3069    -11   -121   -112        C
ATOM   6733  OD1 ASP B 141      77.173  23.463  67.054  1.00 32.27           O
ANISOU 6733  OD1 ASP B 141    4384   3728   4149     95   -202    131        O
ATOM   6734  OD2 ASP B 141      77.141  25.578  66.674  1.00 31.32           O
ANISOU 6734  OD2 ASP B 141    4010   3615   4273   -215     58      4        O
ATOM   6735  C   ASP B 141      74.147  22.745  64.074  1.00 14.19           C
ANISOU 6735  C   ASP B 141    1877   1773   1740    -22      4    -46        C
ATOM   6736  O   ASP B 141      73.111  23.353  64.319  1.00 13.16           O
ANISOU 6736  O   ASP B 141    1857   1656   1485   -151    119   -190        O
ATOM   6737  N   PRO B 142      74.204  21.641  63.323  1.00 11.98           N
ANISOU 6737  N   PRO B 142    1663   1461   1427   -104     -9     41        N
ATOM   6738  CA  PRO B 142      73.001  21.052  62.757  1.00 12.35           C
ANISOU 6738  CA  PRO B 142    1605   1606   1481    -32     29      8        C
ATOM   6740  CB  PRO B 142      73.512  19.793  62.055  1.00 11.69           C
ANISOU 6740  CB  PRO B 142    1607   1437   1396    -23     18     55        C
ATOM   6743  CG  PRO B 142      74.815  19.540  62.654  1.00 12.24           C
ANISOU 6743  CG  PRO B 142    1565   1680   1405   -127     59     -50        C
ATOM   6746  CD  PRO B 142      75.392  20.910  62.912  1.00 11.54           C
ANISOU 6746  CD  PRO B 142    1700   1419   1266   -118    -11     73        C
ATOM   6749  C   PRO B 142      71.975  20.655  63.784  1.00 11.48           C
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ANISOU	6749	C	PRO	B	142	1499	1453	1407	-56	17	59		C
ATOM	6750	O	PRO	B	142	70.808	20.638	63.428	1.00	10.15			O
ANISOU	6750	O	PRO	B	142	1309	1330	1217	-391	-64	-1		O
ATOM	6751	N	GLU	B	143	72.388	20.420	65.023	1.00	11.54			N
ANISOU	6751	N	GLU	B	143	1489	1424	1468	-60	-53	-3		N
ATOM	6753	CA	GLU	B	143	71.448	19.994	66.049	1.00	12.07			C
ANISOU	6753	CA	GLU	B	143	1511	1628	1444	-36	-31	-22		C
ATOM	6755	CB	GLU	B	143	72.171	19.637	67.344	1.00	13.79			C
ANISOU	6755	CB	GLU	B	143	1681	1859	1697	8	49	45		C
ATOM	6758	CG	GLU	B	143	72.826	20.830	67.981	1.00	15.76			C
ANISOU	6758	CG	GLU	B	143	1904	1976	2105	-85	-15	-94		C
ATOM	6761	CD	GLU	B	143	74.214	21.089	67.405	1.00	20.30			C
ANISOU	6761	CD	GLU	B	143	2408	2669	2634	-17	149	13		C
ATOM	6762	OE1	GLU	B	143	74.563	20.444	66.395	1.00	19.55			O
ANISOU	6762	OE1	GLU	B	143	2313	2810	2302	-99	102	87		O
ATOM	6763	OE2	GLU	B	143	74.965	21.903	68.001	1.00	24.75			O
ANISOU	6763	OE2	GLU	B	143	3186	3145	3070	-179	-74	-125		O
ATOM	6764	C	GLU	B	143	70.333	21.009	66.336	1.00	11.68			C
ANISOU	6764	C	GLU	B	143	1624	1457	1354	-44	-30	-53		C
ATOM	6765	O	GLU	B	143	69.352	20.696	66.979	1.00	9.73			O
ANISOU	6765	O	GLU	B	143	1545	1214	936	-107	33	-65		O
ATOM	6766	N	ARG	B	144	70.506	22.240	65.885	1.00	11.97			N
ANISOU	6766	N	ARG	B	144	1794	1593	1160	-36	-19	12		N
ATOM	6768	CA	ARG	B	144	69.509	23.266	66.093	1.00	13.45			C
ANISOU	6768	CA	ARG	B	144	1837	1674	1598	21	-7	37		C
ATOM	6770	CB	ARG	B	144	70.237	24.620	66.071	1.00	15.47			C
ANISOU	6770	CB	ARG	B	144	2137	1886	1855	-1	-38	12		C
ATOM	6773	CG	ARG	B	144	71.340	24.811	67.084	1.00	20.14			C
ANISOU	6773	CG	ARG	B	144	2561	2496	2593	106	-246	-9		C
ATOM	6776	CD	ARG	B	144	72.001	26.227	67.029	1.00	26.90			C
ANISOU	6776	CD	ARG	B	144	3436	3168	3615	-168	-13	63		C
ATOM	6779	NE	ARG	B	144	70.949	27.241	66.875	1.00	31.34			N
ANISOU	6779	NE	ARG	B	144	3967	3791	4149	61	45	97		N
ATOM	6781	CZ	ARG	B	144	70.986	28.287	66.036	1.00	34.22			C
ANISOU	6781	CZ	ARG	B	144	4475	4169	4355	9	73	125		C
ATOM	6782	NH1	ARG	B	144	72.075	28.538	65.266	1.00	32.27			N
ANISOU	6782	NH1	ARG	B	144	4122	3897	4241	-20	78	-1		N
ATOM	6785	NH2	ARG	B	144	69.914	29.089	65.990	1.00	35.63			N
ANISOU	6785	NH2	ARG	B	144	4451	4576	4507	116	108	154		N
ATOM	6788	C	ARG	B	144	68.412	23.304	65.043	1.00	12.87			C
ANISOU	6788	C	ARG	B	144	1792	1596	1503	54	69	42		C
ATOM	6789	O	ARG	B	144	67.444	24.101	65.135	1.00	14.97			O
ANISOU	6789	O	ARG	B	144	2246	1672	1768	257	82	-29		O
ATOM	6790	N	TYR	B	145	68.517	22.441	64.053	1.00	10.68			N
ANISOU	6790	N	TYR	B	145	1475	1237	1344	97	86	31		N
ATOM	6792	CA	TYR	B	145	67.695	22.533	62.849	1.00	10.53			C
ANISOU	6792	CA	TYR	B	145	1291	1382	1329	67	142	-3		C
ATOM	6794	CB	TYR	B	145	68.608	23.026	61.691	1.00	10.83			C
ANISOU	6794	CB	TYR	B	145	1355	1359	1401	-27	114	12		C
ATOM	6797	CG	TYR	B	145	69.032	24.421	61.933	1.00	13.77			C
ANISOU	6797	CG	TYR	B	145	1780	1785	1666	0	58	-15		C
ATOM	6798	CD1	TYR	B	145	70.318	24.714	62.163	1.00	15.65			C
ANISOU	6798	CD1	TYR	B	145	1875	2174	1895	-218	42	-129		C
ATOM	6800	CE1	TYR	B	145	70.727	26.016	62.414	1.00	17.91			C
ANISOU	6800	CE1	TYR	B	145	2408	2055	2342	32	209	-73		C
ATOM	6802	CZ	TYR	B	145	69.822	26.981	62.510	1.00	17.56			C
ANISOU	6802	CZ	TYR	B	145	2159	2294	2219	32	-96	246		C
ATOM	6803	OH	TYR	B	145	70.229	28.234	62.824	1.00	21.30			O
ANISOU	6803	OH	TYR	B	145	2441	2613	3036	-86	99	-8		O
ATOM	6805	CE2	TYR	B	145	68.491	26.723	62.290	1.00	19.02			C
ANISOU	6805	CE2	TYR	B	145	2303	2422	2501	-201	155	9		C

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ATOM   6807  CD2 TYR B 145      68.102  25.442  62.016  1.00 15.32           C
ANISOU 6807  CD2 TYR B 145    1943   1976   1900     74     64   -151       C
ATOM   6809  C   TYR B 145      67.086  21.207  62.443  1.00  9.80           C
ANISOU 6809  C   TYR B 145    1172   1346   1205     45    109    -12       C
ATOM   6810  O   TYR B 145      67.382  20.153  63.035  1.00 10.36           O
ANISOU 6810  O   TYR B 145    1113   1496   1327     55     82     22       O
ATOM   6811  N   GLY B 146      66.245  21.252  61.416  1.00  9.51           N
ANISOU 6811  N   GLY B 146    1090   1219   1303     92     46     97       N
ATOM   6813  CA  GLY B 146      65.809  20.060  60.725  1.00  9.04           C
ANISOU 6813  CA  GLY B 146    1118   1194   1122    125      8     93       C
ATOM   6816  C   GLY B 146      67.071  19.588  59.985  1.00  8.91           C
ANISOU 6816  C   GLY B 146    1065   1171   1148     34     55     97       C
ATOM   6817  O   GLY B 146      67.770  20.401  59.397  1.00  9.39           O
ANISOU 6817  O   GLY B 146    1321   1071   1173     69      8    247       O
ATOM   6818  N   VAL B 147      67.379  18.303  60.031  1.00  7.72           N
ANISOU 6818  N   VAL B 147     910   1078    945    -43     34     53       N
ATOM   6820  CA  VAL B 147      68.588  17.797  59.425  1.00  7.79           C
ANISOU 6820  CA  VAL B 147    1082    909    965     46     25    110       C
ATOM   6822  CB  VAL B 147      69.524  17.185  60.489  1.00  7.20           C
ANISOU 6822  CB  VAL B 147     805    998    933    -24   -110   -105       C
ATOM   6824  CG1 VAL B 147      70.794  16.587  59.878  1.00  6.99           C
ANISOU 6824  CG1 VAL B 147     830    821   1005   -368     69     34       C
ATOM   6828  CG2 VAL B 147      69.781  18.169  61.548  1.00  8.39           C
ANISOU 6828  CG2 VAL B 147    1018   1013   1155    135   -216    -53       C
ATOM   6832  C   VAL B 147      68.245  16.725  58.381  1.00  8.38           C
ANISOU 6832  C   VAL B 147    1009   1190    983    -30    -97     50       C
ATOM   6833  O   VAL B 147      67.457  15.811  58.627  1.00  9.14           O
ANISOU 6833  O   VAL B 147    1233   1203   1036      9      9    118       O
ATOM   6834  N   VAL B 148      68.871  16.843  57.216  1.00  7.84           N
ANISOU 6834  N   VAL B 148     792   1137   1050     10     20     88       N
ATOM   6836  CA  VAL B 148      68.695  15.888  56.162  1.00  8.13           C
ANISOU 6836  CA  VAL B 148     958   1123   1006     27     -4     47       C
ATOM   6838  CB  VAL B 148      68.232  16.534  54.839  1.00  8.35           C
ANISOU 6838  CB  VAL B 148    1031   1112   1027     41    -40     28       C
ATOM   6840  CG1 VAL B 148      69.264  17.584  54.296  1.00  9.93           C
ANISOU 6840  CG1 VAL B 148    1371   1201   1197      0   -119     -2       C
ATOM   6844  CG2 VAL B 148      67.975  15.422  53.760  1.00  9.54           C
ANISOU 6844  CG2 VAL B 148    1275   1213   1135     87    -49    118       C
ATOM   6848  C   VAL B 148      69.972  15.066  55.962  1.00  8.79           C
ANISOU 6848  C   VAL B 148    1135   1173   1030     20      0    -24       C
ATOM   6849  O   VAL B 148      71.100  15.607  55.875  1.00  8.58           O
ANISOU 6849  O   VAL B 148     977   1237   1042     99    -62    -43       O
ATOM   6850  N   GLU B 149      69.769  13.761  55.881  1.00  8.38           N
ANISOU 6850  N   GLU B 149    1104   1038   1039     33    -84     48       N
ATOM   6852  CA  GLU B 149      70.837  12.781  55.604  1.00  8.67           C
ANISOU 6852  CA  GLU B 149    1179   1126    990     82     81      2       C
ATOM   6854  CB  GLU B 149      70.701  11.584  56.570  1.00  8.74           C
ANISOU 6854  CB  GLU B 149    1350   1044    924     70     62     55       C
ATOM   6863  C   GLU B 149      70.737  12.254  54.186  1.00  7.88           C
ANISOU 6863  C   GLU B 149    1057    937    998     34     39     -6       C
ATOM   6864  O   GLU B 149      69.651  12.080  53.659  1.00  7.98           O
ANISOU 6864  O   GLU B 149     866    976   1186    139    238   -174       O
ATOM   6873  CD1 PHE B 150      72.557  14.895  52.134  1.00 12.11           C
ANISOU 6873  CD1 PHE B 150    1643   1428   1531     22   -203     54       C
ATOM   6875  CE1 PHE B 150      72.003  16.216  52.140  1.00 10.64           C
ANISOU 6875  CE1 PHE B 150    1351   1173   1516   -115   -139    -97       C
ATOM   6877  CZ  PHE B 150      71.046  16.534  51.256  1.00 10.18           C
ANISOU 6877  CZ  PHE B 150    1334   1242   1290   -130     40    -33       C
ATOM   6879  CE2 PHE B 150      70.623  15.549  50.351  1.00 11.13           C
ANISOU 6879  CE2 PHE B 150    1491   1469   1268     38   -131   -124       C
ATOM   6881  CD2 PHE B 150      71.171  14.282  50.341  1.00 10.74           C
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ANISOU	6881	CD2	PHE	B	150	1347	1344	1386	-85	-161	29		C
ATOM	6952	CA	ALA	B	156	68.012	12.259	50.637	1.00	13.87			C
ANISOU	6952	CA	ALA	B	156	1728	1857	1685	94	-29	-28		C
ATOM	6954	CB	ALA	B	156	66.884	13.323	50.575	1.00	13.88			C
ANISOU	6954	CB	ALA	B	156	1673	1783	1815	19	-75	-91		C
ATOM	6977	C	ILE	B	157	66.494	9.432	54.217	1.00	13.23			C
ANISOU	6977	C	ILE	B	157	1685	1596	1744	13	146	-106		C
ATOM	6979	N	SER	B	158	66.814	10.480	54.970	1.00	12.13			N
ANISOU	6979	N	SER	B	158	1604	1384	1621	6	127	-37		N
ATOM	6981	CA	SER	B	158	66.092	10.699	56.225	1.00	12.23			C
ANISOU	6981	CA	SER	B	158	1542	1523	1580	30	37	18		C
ATOM	6983	CB	SER	B	158	66.655	9.823	57.342	1.00	12.86			C
ANISOU	6983	CB	SER	B	158	1640	1678	1568	27	39	-24		C
ATOM	6986	OG	SER	B	158	67.745	10.437	57.970	1.00	11.97			O
ANISOU	6986	OG	SER	B	158	1299	1403	1845	20	-59	181		O
ATOM	6988	C	SER	B	158	66.064	12.142	56.642	1.00	10.81			C
ANISOU	6988	C	SER	B	158	1329	1348	1428	52	18	55		C
ATOM	6989	O	SER	B	158	66.892	12.934	56.202	1.00	11.82			O
ANISOU	6989	O	SER	B	158	1345	1578	1567	251	122	56		O
ATOM	6990	N	LEU	B	159	65.088	12.475	57.481	1.00	9.46			N
ANISOU	6990	N	LEU	B	159	1213	1117	1261	-57	64	128		N
ATOM	6992	CA	LEU	B	159	64.879	13.787	58.029	1.00	9.04			C
ANISOU	6992	CA	LEU	B	159	1098	1189	1147	-26	16	82		C
ATOM	6994	CB	LEU	B	159	63.605	14.413	57.398	1.00	8.61			C
ANISOU	6994	CB	LEU	B	159	969	1151	1151	-97	79	188		C
ATOM	6997	CG	LEU	B	159	63.761	14.649	55.868	1.00	10.31			C
ANISOU	6997	CG	LEU	B	159	1332	1409	1174	-50	-118	25		C
ATOM	6999	CD1	LEU	B	159	62.421	15.004	55.226	1.00	12.39			C
ANISOU	6999	CD1	LEU	B	159	1511	1595	1602	-8	-35	227		C
ATOM	7003	CD2	LEU	B	159	64.708	15.846	55.696	1.00	13.41			C
ANISOU	7003	CD2	LEU	B	159	1552	1838	1705	-57	71	214		C
ATOM	7007	C	LEU	B	159	64.660	13.645	59.520	1.00	8.85			C
ANISOU	7007	C	LEU	B	159	1084	1147	1129	-8	-25	45		C
ATOM	7008	O	LEU	B	159	63.891	12.786	59.942	1.00	7.91			O
ANISOU	7008	O	LEU	B	159	1140	1062	803	-123	13	29		O
ATOM	7009	N	GLU	B	160	65.332	14.476	60.310	1.00	8.63			N
ANISOU	7009	N	GLU	B	160	1081	1059	1136	36	-25	69		N
ATOM	7011	CA	GLU	B	160	65.158	14.493	61.739	1.00	8.95			C
ANISOU	7011	CA	GLU	B	160	1115	1153	1130	72	-16	-32		C
ATOM	7013	CB	GLU	B	160	66.331	13.815	62.438	1.00	7.85			C
ANISOU	7013	CB	GLU	B	160	987	1021	973	64	71	39		C
ATOM	7016	CG	GLU	B	160	66.390	12.339	62.103	1.00	9.92			C
ANISOU	7016	CG	GLU	B	160	1125	1167	1477	-157	-37	38		C
ATOM	7019	CD	GLU	B	160	67.368	11.600	62.960	1.00	13.56			C
ANISOU	7019	CD	GLU	B	160	1471	1568	2110	-16	-165	141		C
ATOM	7020	OE1	GLU	B	160	68.420	12.139	63.361	1.00	11.79			O
ANISOU	7020	OE1	GLU	B	160	1364	1270	1843	114	25	-131		O
ATOM	7021	OE2	GLU	B	160	67.066	10.458	63.251	1.00	19.57			O
ANISOU	7021	OE2	GLU	B	160	2555	2049	2830	-104	-202	256		O
ATOM	7022	C	GLU	B	160	65.073	15.953	62.223	1.00	9.19			C
ANISOU	7022	C	GLU	B	160	1198	1123	1170	109	2	46		C
ATOM	7023	O	GLU	B	160	65.847	16.795	61.801	1.00	8.81			O
ANISOU	7023	O	GLU	B	160	1165	1090	1091	224	183	-91		O
ATOM	7024	N	GLU	B	161	64.105	16.230	63.101	1.00	7.95			N
ANISOU	7024	N	GLU	B	161	945	1136	939	63	6	108		N
ATOM	7026	CA	GLU	B	161	64.002	17.544	63.679	1.00	9.71			C
ANISOU	7026	CA	GLU	B	161	1269	1335	1083	73	-29	54		C
ATOM	7028	CB	GLU	B	161	62.541	17.931	63.962	1.00	10.03			C
ANISOU	7028	CB	GLU	B	161	1296	1308	1204	6	-27	34		C
ATOM	7031	CG	GLU	B	161	62.378	19.345	64.548	1.00	11.96			C
ANISOU	7031	CG	GLU	B	161	1668	1525	1351	68	109	21		C

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ATOM   7034  CD  GLU B 161      62.621  20.471  63.580  1.00 10.40           C
ANISOU 7034  CD  GLU B 161    1366   1297   1288     77   -121    -23       C
ATOM   7035  OE1 GLU B 161      62.769  20.217  62.344  1.00  9.46           O
ANISOU 7035  OE1 GLU B 161    1144   1335   1113    315    -17    200       O
ATOM   7036  OE2 GLU B 161      62.698  21.630  64.081  1.00 11.19           O
ANISOU 7036  OE2 GLU B 161    1685   1516   1049    162   -158    -49       O
ATOM   7037  C   GLU B 161      64.831  17.672  64.977  1.00  9.61           C
ANISOU 7037  C   GLU B 161    1198   1288   1165     73    -60     48       C
ATOM   7038  O   GLU B 161      64.547  17.017  65.990  1.00  9.49           O
ANISOU 7038  O   GLU B 161    1036   1659    907    123   -157     48       O
ATOM   7039  N   LYS B 162      65.769  18.585  64.932  1.00  8.24           N
ANISOU 7039  N   LYS B 162     900   1202   1027    135    112      32       N
ATOM   7041  CA  LYS B 162      66.612  18.922  66.038  1.00 10.61           C
ANISOU 7041  CA  LYS B 162    1414   1348   1266     51     54     15       C
ATOM   7043  CB  LYS B 162      65.777  19.741  67.040  1.00 11.54           C
ANISOU 7043  CB  LYS B 162    1456   1471   1456    102     -6     36       C
ATOM   7046  CG  LYS B 162      65.558  21.165  66.523  1.00 15.09           C
ANISOU 7046  CG  LYS B 162    1991   1686   2055    126    -46     54       C
ATOM   7049  CD  LYS B 162      64.544  21.836  67.435  1.00 17.98           C
ANISOU 7049  CD  LYS B 162    2270   2386   2175    120     89    -28       C
ATOM   7052  CE  LYS B 162      63.865  23.039  66.780  1.00 19.21           C
ANISOU 7052  CE  LYS B 162    2468   2383   2447    120     47    101       C
ATOM   7055  NZ  LYS B 162      64.917  23.948  66.384  1.00 25.24           N
ANISOU 7055  NZ  LYS B 162    3210   2930   3447     -1     42     78       N
ATOM   7059  C   LYS B 162      67.227  17.716  66.718  1.00 11.03           C
ANISOU 7059  C   LYS B 162    1314   1513   1364    144     45      6       C
ATOM   7060  O   LYS B 162      67.126  17.581  67.951  1.00 11.36           O
ANISOU 7060  O   LYS B 162    1530   1578   1206    230    217    -21       O
ATOM   7061  N   PRO B 163      67.881  16.837  65.949  1.00 10.90           N
ANISOU 7061  N   PRO B 163    1369   1469   1300      5     62    -12       N
ATOM   7062  CA  PRO B 163      68.501  15.646  66.534  1.00 10.11           C
ANISOU 7062  CA  PRO B 163    1179   1379   1283     20    102     16       C
ATOM   7064  CB  PRO B 163      68.952  14.853  65.303  1.00 10.34           C
ANISOU 7064  CB  PRO B 163    1335   1295   1296   -121    -21    -45       C
ATOM   7067  CG  PRO B 163      69.193  15.867  64.337  1.00 11.48           C
ANISOU 7067  CG  PRO B 163    1511   1580   1269      9    -12     48       C
ATOM   7070  CD  PRO B 163      68.085  16.867  64.494  1.00 10.62           C
ANISOU 7070  CD  PRO B 163    1190   1536   1306    -21    149     22       C
ATOM   7073  C   PRO B 163      69.682  15.923  67.453  1.00  9.77           C
ANISOU 7073  C   PRO B 163    1237   1212   1262    -68     74    -20       C
ATOM   7074  O   PRO B 163      70.536  16.755  67.176  1.00  8.05           O
ANISOU 7074  O   PRO B 163     638   1151   1270     31     86    163       O
ATOM   7075  N   LEU B 164      69.704  15.244  68.586  1.00  9.04           N
ANISOU 7075  N   LEU B 164    1196   1040   1196     37     53     -2       N
ATOM   7077  CA  LEU B 164      70.811  15.393  69.491  1.00 11.39           C
ANISOU 7077  CA  LEU B 164    1511   1363   1453      7     34    -10       C
ATOM   7079  CB  LEU B 164      70.523  14.622  70.770  1.00 12.96           C
ANISOU 7079  CB  LEU B 164    1722   1676   1525     20     43      8       C
ATOM   7082  CG  LEU B 164      69.397  15.097  71.678  1.00 17.24           C
ANISOU 7082  CG  LEU B 164    2118   2230   2201     89     70    -32       C
ATOM   7084  CD1 LEU B 164      69.777  14.694  73.107  1.00 20.27           C
ANISOU 7084  CD1 LEU B 164    2686   2662   2351    -51    -52    -87       C
ATOM   7088  CD2 LEU B 164      69.152  16.549  71.571  1.00 20.80           C
ANISOU 7088  CD2 LEU B 164    2721   2523   2659     -3    125    -15       C
ATOM   7092  C   LEU B 164      72.106  14.910  68.853  1.00 10.34           C
ANISOU 7092  C   LEU B 164    1309   1312   1306      0     58     28       C
ATOM   7093  O   LEU B 164      73.202  15.461  69.140  1.00 11.48           O
ANISOU 7093  O   LEU B 164    1825   1369   1164    -68   -124   -274       O
ATOM   7094  N   GLU B 165      72.014  13.917  67.981  1.00  9.08           N
ANISOU 7094  N   GLU B 165     983   1208   1257   -135      7    -17       N
ATOM   7096  CA  GLU B 165      73.208  13.371  67.248  1.00 10.89           C
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ANISOU 7096  CA  GLU B 165     1475   1357   1304      6     32      0       C
ATOM   7107  C   GLU B 165      72.803  13.407  65.771  1.00 10.15           C
ANISOU 7107  C   GLU B 165     1363   1274   1219    -38     11     -4       C
ATOM   7108  O   GLU B 165      72.297  12.454  65.194  1.00  9.49           O
ANISOU 7108  O   GLU B 165     1186   1135   1282    -92     64     18       O
ATOM   7109  N   PRO B 166      73.017  14.558  65.180  1.00  9.27           N
ANISOU 7109  N   PRO B 166     1240   1180   1101    -12     34      2       N
ATOM   7110  CA  PRO B 166      72.707  14.753  63.767  1.00  8.50           C
ANISOU 7110  CA  PRO B 166     1016   1168   1045      6    -19     35       C
ATOM   7112  CB  PRO B 166      73.184  16.161  63.479  1.00  8.60           C
ANISOU 7112  CB  PRO B 166     1047   1184   1034    -39      6    -54       C
ATOM   7115  CG  PRO B 166      73.454  16.820  64.802  1.00 10.24           C
ANISOU 7115  CG  PRO B 166     1479   1335   1076    -97     23     16       C
ATOM   7118  CD  PRO B 166      73.566  15.741  65.851  1.00  9.86           C
ANISOU 7118  CD  PRO B 166     1331   1166   1248    -10    -66     38       C
ATOM   7121  C   PRO B 166      73.433  13.769  62.861  1.00  8.82           C
ANISOU 7121  C   PRO B 166     1090   1200   1058     -9      7     57       C
ATOM   7122  O   PRO B 166      74.650  13.478  63.053  1.00  9.73           O
ANISOU 7122  O   PRO B 166     1035   1533   1128    148    169     21       O
ATOM   7123  N   LYS B 167      72.711  13.280  61.860  1.00  8.94           N
ANISOU 7123  N   LYS B 167     1119   1142   1135    -82    210     54       N
ATOM   7125  CA  LYS B 167      73.279  12.330  60.928  1.00  9.63           C
ANISOU 7125  CA  LYS B 167     1278   1123   1258     39     90    -27       C
ATOM   7127  CB  LYS B 167      72.183  11.470  60.289  1.00  8.15           C
ANISOU 7127  CB  LYS B 167      960   1010   1126    111    128   -110       C
ATOM   7130  CG  LYS B 167      71.617  10.439  61.327  1.00 11.24           C
ANISOU 7130  CG  LYS B 167     1544   1370   1354     94    112    -31       C
ATOM   7133  CD  LYS B 167      70.366   9.721  60.827  1.00 13.95           C
ANISOU 7133  CD  LYS B 167     1691   1784   1825     -4     49    -54       C
ATOM   7143  C   LYS B 167      74.144  12.979  59.848  1.00  8.82           C
ANISOU 7143  C   LYS B 167     1025   1081   1244     -1     88    -20       C
ATOM   7144  O   LYS B 167      74.781  12.256  59.092  1.00 10.84           O
ANISOU 7144  O   LYS B 167     1677   1095   1344     24    131    -56       O
ATOM   7145  N   SER B 168      74.090  14.317  59.728  1.00  7.84           N
ANISOU 7145  N   SER B 168      858   1062   1056    -27    -62     32       N
ATOM   7147  CA  SER B 168      74.913  15.048  58.788  1.00  8.49           C
ANISOU 7147  CA  SER B 168      964   1151   1110      2    -31    -32       C
ATOM   7149  CB  SER B 168      74.321  15.086  57.392  1.00  7.62           C
ANISOU 7149  CB  SER B 168      888   1013    992    -25    -44   -109       C
ATOM   7152  OG  SER B 168      73.281  16.077  57.307  1.00  8.98           O
ANISOU 7152  OG  SER B 168      826   1444   1140     53   -406   -271       O
ATOM   7154  C   SER B 168      75.000  16.498  59.258  1.00  8.20           C
ANISOU 7154  C   SER B 168      925   1116   1075     27    -72    -66       C
ATOM   7155  O   SER B 168      74.394  16.864  60.255  1.00  9.84           O
ANISOU 7155  O   SER B 168     1046   1365   1325   -134      2   -118       O
ATOM   7156  N   ASN B 169      75.720  17.311  58.516  1.00  8.34           N
ANISOU 7156  N   ASN B 169     1082   1134    953     33    -28     12       N
ATOM   7158  CA  ASN B 169      75.830  18.723  58.792  1.00  9.44           C
ANISOU 7158  CA  ASN B 169     1280   1219   1087     60     21    -29       C
ATOM   7160  CB  ASN B 169      77.288  19.190  58.675  1.00 10.02           C
ANISOU 7160  CB  ASN B 169     1439   1222   1145      1    -50    -65       C
ATOM   7163  CG  ASN B 169      78.135  18.686  59.862  1.00 11.94           C
ANISOU 7163  CG  ASN B 169     1572   1549   1415     80   -166   -103       C
ATOM   7164  OD1 ASN B 169      77.697  18.777  61.022  1.00 16.26           O
ANISOU 7164  OD1 ASN B 169     2408   2285   1485     95   -122    102       O
ATOM   7165  ND2 ASN B 169      79.280  18.144  59.581  1.00 10.28           N
ANISOU 7165  ND2 ASN B 169     1387   1439   1079      3   -271    -63       N
ATOM   7168  C   ASN B 169      74.902  19.558  57.911  1.00  9.68           C
ANISOU 7168  C   ASN B 169     1384   1215   1077    -22    -80    -15       C
ATOM   7169  O   ASN B 169      75.076  20.779  57.793  1.00 10.98           O
ANISOU 7169  O   ASN B 169     1808   1180   1180   -171    -94    -73       O
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ATOM   7170  N   TYR B 170      73.947  18.924  57.249  1.00  8.76           N
ANISOU 7170  N   TYR B 170    1193   1035   1100    -16    82    -62       N
ATOM   7172  CA  TYR B 170      73.041  19.648  56.357  1.00  6.97           C
ANISOU 7172  CA  TYR B 170     859    947    839    -65    20    -13       C
ATOM   7174  CB  TYR B 170      72.838  18.873  55.047  1.00  7.14           C
ANISOU 7174  CB  TYR B 170     744   1100    869     27    64    -56       C
ATOM   7177  CG  TYR B 170      74.049  19.087  54.169  1.00  6.20           C
ANISOU 7177  CG  TYR B 170     682    865    806    -82    28     84       C
ATOM   7178  CD1 TYR B 170      75.125  18.210  54.227  1.00  7.09           C
ANISOU 7178  CD1 TYR B 170     881   1015    797    -42   -24    -21       C
ATOM   7180  CE1 TYR B 170      76.267  18.445  53.502  1.00  6.23           C
ANISOU 7180  CE1 TYR B 170     789    825    751    -21    92    -81       C
ATOM   7182  CZ  TYR B 170      76.319  19.611  52.703  1.00  8.76           C
ANISOU 7182  CZ  TYR B 170    1264   1229    833    -31  -143    -45       C
ATOM   7185  CE2 TYR B 170      75.288  20.489  52.678  1.00  8.94           C
ANISOU 7185  CE2 TYR B 170    1111   1124   1159    -72   148    -78       C
ATOM   7187  CD2 TYR B 170      74.161  20.230  53.421  1.00  7.63           C
ANISOU 7187  CD2 TYR B 170    1007    924    965    -99    42    -17       C
ATOM   7189  C   TYR B 170      71.705  19.966  56.998  1.00  8.15           C
ANISOU 7189  C   TYR B 170     980   1052   1062    -14     4     -7       C
ATOM   7190  O   TYR B 170      70.939  19.041  57.332  1.00  9.22           O
ANISOU 7190  O   TYR B 170    1159   1096   1248   -254   192    159       O
ATOM   7191  N   ALA B 171      71.437  21.251  57.213  1.00  7.85           N
ANISOU 7191  N   ALA B 171     922    915   1145    -85    -3    128       N
ATOM   7193  CA  ALA B 171      70.157  21.703  57.779  1.00  6.04           C
ANISOU 7193  CA  ALA B 171     830    722    741    -16    -7    129       C
ATOM   7195  CB  ALA B 171      70.345  23.032  58.562  1.00  7.20           C
ANISOU 7195  CB  ALA B 171     910    977    845     34  -101    113       C
ATOM   7199  C   ALA B 171      69.182  21.939  56.641  1.00  7.69           C
ANISOU 7199  C   ALA B 171     914   1065    940    -10   -11     60       C
ATOM   7200  O   ALA B 171      69.585  22.371  55.569  1.00  9.49           O
ANISOU 7200  O   ALA B 171    1245   1401    958     41   -59     75       O
ATOM   7201  N   VAL B 172      67.904  21.754  56.929  1.00  7.02           N
ANISOU 7201  N   VAL B 172     877    941    849    -86    37     83       N
ATOM   7203  CA  VAL B 172      66.820  22.038  55.994  1.00  7.98           C
ANISOU 7203  CA  VAL B 172     986   1067    978     -7    60     93       C
ATOM   7205  CB  VAL B 172      65.689  21.006  56.048  1.00  7.69           C
ANISOU 7205  CB  VAL B 172     860    985   1074     13    10     81       C
ATOM   7207  CG1 VAL B 172      64.547  21.391  55.088  1.00  7.84           C
ANISOU 7207  CG1 VAL B 172    1162   1028    787   -190   -64    125       C
ATOM   7211  CG2 VAL B 172      66.192  19.558  55.778  1.00  8.46           C
ANISOU 7211  CG2 VAL B 172    1103   1224    887   -156   204    -81       C
ATOM   7215  C   VAL B 172      66.365  23.443  56.381  1.00  8.06           C
ANISOU 7215  C   VAL B 172     967   1038   1058    -44     8     38       C
ATOM   7216  O   VAL B 172      65.849  23.672  57.484  1.00  7.37           O
ANISOU 7216  O   VAL B 172     858    896   1044      0  -160    147       O
ATOM   7217  N   THR B 173      66.585  24.394  55.469  1.00  9.20           N
ANISOU 7217  N   THR B 173    1211   1258   1024     32    28     12       N
ATOM   7219  CA  THR B 173      66.371  25.812  55.744  1.00  9.64           C
ANISOU 7219  CA  THR B 173    1185   1226   1249     26    17     75       C
ATOM   7221  CB  THR B 173      67.023  26.735  54.707  1.00  9.14           C
ANISOU 7221  CB  THR B 173    1041   1285   1147     96   122     -4       C
ATOM   7223  OG1 THR B 173      66.266  26.732  53.499  1.00 10.36           O
ANISOU 7223  OG1 THR B 173    1012   1431   1493    -10   304     28       O
ATOM   7225  CG2 THR B 173      68.470  26.306  54.352  1.00 10.18           C
ANISOU 7225  CG2 THR B 173    1304   1372   1190    -76   229    162       C
ATOM   7229  C   THR B 173      64.866  26.124  55.842  1.00  8.67           C
ANISOU 7229  C   THR B 173    1013   1152   1126     44    72     68       C
ATOM   7230  O   THR B 173      64.072  25.302  55.440  1.00  9.73           O
ANISOU 7230  O   THR B 173    1318   1015   1363    113   -24     71       O
ATOM   7231  N   GLY B 174      64.521  27.335  56.293  1.00  9.12           N
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ANISOU	7231	N	GLY	B	174	1083	1193	1187	-43	-31	16		N
ATOM	7233	CA	GLY	B	174	63.118	27.788	56.507	1.00	8.23			C
ANISOU	7233	CA	GLY	B	174	998	908	1220	-40	-25	-18		C
ATOM	7236	C	GLY	B	174	62.455	28.303	55.233	1.00	8.36			C
ANISOU	7236	C	GLY	B	174	950	962	1263	-58	-50	-3		C
ATOM	7237	O	GLY	B	174	61.864	29.391	55.196	1.00	9.09			O
ANISOU	7237	O	GLY	B	174	902	1011	1540	-22	-184	-212		O
ATOM	7238	N	LEU	B	175	62.550	27.547	54.168	1.00	8.58			N
ANISOU	7238	N	LEU	B	175	1052	932	1275	102	-60	-34		N
ATOM	7240	CA	LEU	B	175	61.951	27.902	52.868	1.00	9.59			C
ANISOU	7240	CA	LEU	B	175	1235	1096	1313	37	33	-36		C
ATOM	7242	CB	LEU	B	175	62.951	28.584	51.975	1.00	9.42			C
ANISOU	7242	CB	LEU	B	175	1080	1117	1381	-85	-51	-70		C
ATOM	7245	CG	LEU	B	175	62.330	28.947	50.646	1.00	11.58			C
ANISOU	7245	CG	LEU	B	175	1567	1326	1505	60	111	-63		C
ATOM	7247	CD1	LEU	B	175	61.151	29.961	50.721	1.00	8.89			C
ANISOU	7247	CD1	LEU	B	175	759	1276	1341	-262	58	54		C
ATOM	7251	CD2	LEU	B	175	63.498	29.481	49.870	1.00	12.70			C
ANISOU	7251	CD2	LEU	B	175	1717	1586	1521	-282	120	-139		C
ATOM	7255	C	LEU	B	175	61.462	26.629	52.196	1.00	8.98			C
ANISOU	7255	C	LEU	B	175	1141	1076	1194	10	33	-71		C
ATOM	7256	O	LEU	B	175	62.238	25.714	52.008	1.00	10.88			O
ANISOU	7256	O	LEU	B	175	1319	1383	1430	24	167	-204		O
ATOM	7257	N	TYR	B	176	60.183	26.555	51.939	1.00	7.28			N
ANISOU	7257	N	TYR	B	176	905	773	1086	106	46	-100		N
ATOM	7259	CA	TYR	B	176	59.497	25.326	51.518	1.00	8.16			C
ANISOU	7259	CA	TYR	B	176	916	997	1185	37	102	-9		C
ATOM	7261	CB	TYR	B	176	58.786	24.724	52.739	1.00	7.87			C
ANISOU	7261	CB	TYR	B	176	937	899	1154	-8	-36	100		C
ATOM	7264	CG	TYR	B	176	59.526	24.715	54.008	1.00	7.97			C
ANISOU	7264	CG	TYR	B	176	991	841	1196	-64	-12	-29		C
ATOM	7265	CD1	TYR	B	176	59.388	25.734	54.907	1.00	9.89			C
ANISOU	7265	CD1	TYR	B	176	1240	1304	1213	268	120	2		C
ATOM	7267	CE1	TYR	B	176	60.079	25.737	56.091	1.00	8.98			C
ANISOU	7267	CE1	TYR	B	176	815	1243	1353	35	-113	-69		C
ATOM	7269	CZ	TYR	B	176	60.968	24.694	56.398	1.00	8.89			C
ANISOU	7269	CZ	TYR	B	176	988	1207	1182	69	32	27		C
ATOM	7270	OH	TYR	B	176	61.655	24.705	57.632	1.00	7.40			O
ANISOU	7270	OH	TYR	B	176	372	1252	1185	-104	32	178		O
ATOM	7272	CE2	TYR	B	176	61.147	23.683	55.518	1.00	7.38			C
ANISOU	7272	CE2	TYR	B	176	451	1022	1331	-294	-21	-15		C
ATOM	7274	CD2	TYR	B	176	60.485	23.705	54.295	1.00	8.70			C
ANISOU	7274	CD2	TYR	B	176	1083	1052	1167	9	-55	139		C
ATOM	7276	C	TYR	B	176	58.472	25.580	50.419	1.00	7.85			C
ANISOU	7276	C	TYR	B	176	1068	896	1017	-52	111	23		C
ATOM	7277	O	TYR	B	176	57.621	26.490	50.539	1.00	8.80			O
ANISOU	7277	O	TYR	B	176	1127	1079	1138	34	154	26		O
ATOM	7278	N	PHE	B	177	58.536	24.797	49.335	1.00	7.19			N
ANISOU	7278	N	PHE	B	177	1047	787	896	-43	75	2		N
ATOM	7280	CA	PHE	B	177	57.627	24.921	48.216	1.00	7.33			C
ANISOU	7280	CA	PHE	B	177	818	932	1032	3	46	-7		C
ATOM	7282	CB	PHE	B	177	58.419	25.078	46.915	1.00	7.10			C
ANISOU	7282	CB	PHE	B	177	974	939	781	-67	-115	62		C
ATOM	7285	CG	PHE	B	177	59.066	26.422	46.767	1.00	7.98			C
ANISOU	7285	CG	PHE	B	177	959	973	1100	-118	-151	-43		C
ATOM	7286	CD1	PHE	B	177	60.281	26.688	47.384	1.00	8.17			C
ANISOU	7286	CD1	PHE	B	177	724	1045	1335	12	-101	-84		C
ATOM	7288	CE1	PHE	B	177	60.852	27.910	47.240	1.00	9.74			C
ANISOU	7288	CE1	PHE	B	177	896	1193	1610	-64	-197	-26		C
ATOM	7290	CZ	PHE	B	177	60.242	28.929	46.525	1.00	10.02			C
ANISOU	7290	CZ	PHE	B	177	1083	1433	1288	-135	-83	144		C

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ATOM   7296  C   PHE B 177      56.769  23.644  48.140  1.00  7.12           C
ANISOU 7296  C   PHE B 177       967    821    915     39     12   -138      C
ATOM   7297  O   PHE B 177      57.318  22.531  48.200  1.00  8.86           O
ANISOU 7297  O   PHE B 177      1163   1024   1177    162   -173   -113      O
ATOM   7298  N   TYR B 178      55.438  23.808  48.103  1.00  5.89           N
ANISOU 7298  N   TYR B 178       673    838    726     40   -204   -154      N
ATOM   7302  CB  TYR B 178      53.773  22.537  49.407  1.00  8.00           C
ANISOU 7302  CB  TYR B 178      1075    946   1017     91     45    -20      C
ATOM   7305  CG  TYR B 178      54.683  22.338  50.579  1.00  6.73           C
ANISOU 7305  CG  TYR B 178       590   1082    885    -94    167     42      C
ATOM   7306  CD1 TYR B 178      54.890  23.343  51.492  1.00  8.96           C
ANISOU 7306  CD1 TYR B 178       842   1200   1362    161     26     33      C
ATOM   7308  CE1 TYR B 178      55.685  23.176  52.554  1.00  7.92           C
ANISOU 7308  CE1 TYR B 178      1075   1280    653     45    174    -51      C
ATOM   7310  CZ  TYR B 178      56.347  21.956  52.733  1.00  9.90           C
ANISOU 7310  CZ  TYR B 178      1269   1275   1216    -62     47    -48      C
ATOM   7311  OH  TYR B 178      57.152  21.787  53.814  1.00 11.41           O
ANISOU 7311  OH  TYR B 178      1388   1768   1175    241    -23      8      O
ATOM   7313  CE2 TYR B 178      56.175  20.933  51.836  1.00 10.09           C
ANISOU 7313  CE2 TYR B 178      1238   1289   1305    -31     -3    -55      C
ATOM   7315  CD2 TYR B 178      55.317  21.143  50.756  1.00  7.48           C
ANISOU 7315  CD2 TYR B 178       803    969   1067   -285    218     96      C
ATOM   7375  CG2 VAL B 182      51.971  21.111  52.994  1.00  8.00           C
ANISOU 7375  CG2 VAL B 182       546   1403   1087    -54    -64     83      C
ATOM   7422  CG2 ILE B 185      51.599  16.073  55.179  1.00 12.67           C
ANISOU 7422  CG2 ILE B 185      1651   1554   1609    110    -11    -97      C
ATOM   7428  N   ALA B 186      49.151  18.085  56.330  1.00 10.77           N
ANISOU 7428  N   ALA B 186      1360   1340   1389      4    -98    -48      N
ATOM   7430  CA  ALA B 186      49.169  18.840  57.574  1.00 11.68           C
ANISOU 7430  CA  ALA B 186      1479   1473   1484      8    -31     -4      C
ATOM   7432  CB  ALA B 186      49.225  20.346  57.254  1.00 11.61           C
ANISOU 7432  CB  ALA B 186      1626   1449   1335     45      6   -194      C
ATOM   7436  C   ALA B 186      47.988  18.476  58.461  1.00 12.71           C
ANISOU 7436  C   ALA B 186      1674   1579   1575     28     16    -47      C
ATOM   7437  O   ALA B 186      48.149  18.327  59.678  1.00 12.14           O
ANISOU 7437  O   ALA B 186      1516   1560   1538    -30    -15    -18      O
ATOM   7438  N   ARG B 187      46.842  18.242  57.825  1.00 13.18           N
ANISOU 7438  N   ARG B 187      1625   1686   1695    -19    -23     16      N
ATOM   7474  N   LEU B 189      48.515  15.399  60.551  1.00 16.10           N
ANISOU 7474  N   LEU B 189      2063   2029   2025    -81     98     63      N
ATOM   7476  CA  LEU B 189      49.577  15.457  61.549  1.00 16.49           C
ANISOU 7476  CA  LEU B 189      2101   2072   2091    -53      6     33      C
ATOM   7478  CB  LEU B 189      50.490  16.644  61.274  1.00 16.83           C
ANISOU 7478  CB  LEU B 189      2170   2105   2117    -22      8     79      C
ATOM   7481  CG  LEU B 189      51.338  16.526  60.036  1.00 18.75           C
ANISOU 7481  CG  LEU B 189      2537   2344   2243     22     34     41      C
ATOM   7483  CD1 LEU B 189      52.315  17.642  60.087  1.00 20.29           C
ANISOU 7483  CD1 LEU B 189      2490   2703   2517    -87    -45     39      C
ATOM   7487  CD2 LEU B 189      52.052  15.217  59.871  1.00 19.13           C
ANISOU 7487  CD2 LEU B 189      2221   2547   2498    103      0     85      C
ATOM   7491  C   LEU B 189      49.075  15.546  63.004  1.00 16.86           C
ANISOU 7491  C   LEU B 189      2192   2091   2122    -52     27    -25      C
ATOM   7492  O   LEU B 189      47.990  16.075  63.292  1.00 16.15           O
ANISOU 7492  O   LEU B 189      2169   2171   1795   -229    210     30      O
ATOM   7493  N   LYS B 190      49.883  14.966  63.876  1.00 17.97           N
ANISOU 7493  N   LYS B 190      2412   2211   2202    -56    -47    -57      N
ATOM   7495  CA  LYS B 190      49.706  15.010  65.308  1.00 19.53           C
ANISOU 7495  CA  LYS B 190      2539   2433   2448    -42     48     19      C
ATOM   7513  C   LYS B 190      50.967  15.681  65.884  1.00 19.71           C
ANISOU 7513  C   LYS B 190      2529   2527   2433     10    -18     39      C
ATOM   7514  O   LYS B 190      52.050  15.627  65.306  1.00 18.46           O
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ANISOU 7514  O   LYS B 190     2348   2216   2447     46    -19      6       O
ATOM   7515  N   PRO B 191      50.837  16.297  67.037  1.00 20.60           N
ANISOU 7515  N   PRO B 191     2647   2543   2636     18      4    -38       N
ATOM   7516  CA  PRO B 191      51.992  16.922  67.667  1.00 20.66           C
ANISOU 7516  CA  PRO B 191     2546   2636   2665    -25     31    -13       C
ATOM   7518  CB  PRO B 191      51.443  17.431  68.993  1.00 21.14           C
ANISOU 7518  CB  PRO B 191     2673   2788   2568    -27    -13     43       C
ATOM   7521  CG  PRO B 191      49.990  17.490  68.831  1.00 20.59           C
ANISOU 7521  CG  PRO B 191     2543   2680   2597      0     31      8       C
ATOM   7524  CD  PRO B 191      49.629  16.407  67.876  1.00 20.66           C
ANISOU 7524  CD  PRO B 191     2619   2631   2598    -21     44     14       C
ATOM   7527  C   PRO B 191      53.109  15.954  67.936  1.00 20.82           C
ANISOU 7527  C   PRO B 191     2686   2586   2636    -36      8     43       C
ATOM   7528  O   PRO B 191      52.888  14.802  68.281  1.00 20.54           O
ANISOU 7528  O   PRO B 191     2721   2529   2551   -233     97     63       O
ATOM   7529  N   SER B 192      54.334  16.452  67.791  1.00 20.18           N
ANISOU 7529  N   SER B 192     2515   2559   2592    -49      4     32       N
ATOM   7531  CA  SER B 192      55.522  15.645  68.009  1.00 20.49           C
ANISOU 7531  CA  SER B 192     2640   2562   2581    -12    -12     41       C
ATOM   7533  CB  SER B 192      56.676  16.336  67.312  1.00 20.07           C
ANISOU 7533  CB  SER B 192     2586   2530   2508     35    -27    -21       C
ATOM   7536  OG  SER B 192      56.924  17.600  67.915  1.00 16.60           O
ANISOU 7536  OG  SER B 192     2175   1953   2177     12    -75    238       O
ATOM   7538  C   SER B 192      55.853  15.576  69.503  1.00 22.31           C
ANISOU 7538  C   SER B 192     2911   2820   2745     11     10     20       C
ATOM   7539  O   SER B 192      55.197  16.183  70.328  1.00 22.56           O
ANISOU 7539  O   SER B 192     3054   2894   2621    -49    120    130       O
ATOM   7540  N   PRO B 193      56.902  14.864  69.845  1.00 23.94           N
ANISOU 7540  N   PRO B 193     3070   3054   2971     40    -40     16       N
ATOM   7541  CA  PRO B 193      57.349  14.879  71.229  1.00 25.06           C
ANISOU 7541  CA  PRO B 193     3188   3203   3128     20    -21     -8       C
ATOM   7543  CB  PRO B 193      58.548  13.935  71.219  1.00 25.63           C
ANISOU 7543  CB  PRO B 193     3310   3260   3164     53    -43     -6       C
ATOM   7546  CG  PRO B 193      58.433  13.132  69.969  1.00 25.15           C
ANISOU 7546  CG  PRO B 193     3262   3149   3144     15    -75     35       C
ATOM   7549  CD  PRO B 193      57.732  14.009  68.980  1.00 24.02           C
ANISOU 7549  CD  PRO B 193     3047   3038   3040     20    -32     49       C
ATOM   7552  C   PRO B 193      57.709  16.352  71.624  1.00 25.81           C
ANISOU 7552  C   PRO B 193     3309   3289   3207     19      7      2       C
ATOM   7553  O   PRO B 193      57.427  16.755  72.732  1.00 27.82           O
ANISOU 7553  O   PRO B 193     3603   3576   3388    100   -107   -123       O
ATOM   7554  N   ARG B 194      58.272  17.162  70.734  1.00 25.10           N
ANISOU 7554  N   ARG B 194     3178   3155   3204      9    -29     -2       N
ATOM   7556  CA  ARG B 194      58.520  18.563  71.066  1.00 24.00           C
ANISOU 7556  CA  ARG B 194     3013   3039   3065     47    -20     -6       C
ATOM   7558  CB  ARG B 194      59.263  19.245  69.910  1.00 23.37           C
ANISOU 7558  CB  ARG B 194     3000   2954   2923     22    -39    -13       C
ATOM   7561  CG  ARG B 194      60.797  19.042  69.907  1.00 24.76           C
ANISOU 7561  CG  ARG B 194     3153   3109   3144     -7     32     -2       C
ATOM   7564  CD  ARG B 194      61.541  19.205  68.503  1.00 28.11           C
ANISOU 7564  CD  ARG B 194     3686   3508   3487     44     98     88       C
ATOM   7567  NE  ARG B 194      62.228  17.946  68.264  1.00 28.35           N
ANISOU 7567  NE  ARG B 194     3706   3686   3377    -25     76    -27       N
ATOM   7569  CZ  ARG B 194      61.689  16.907  67.652  1.00 25.85           C
ANISOU 7569  CZ  ARG B 194     3267   3480   3074    -14     44    -16       C
ATOM   7570  NH1 ARG B 194      60.494  16.982  67.031  1.00 22.00           N
ANISOU 7570  NH1 ARG B 194     2562   3096   2700     39    326    308       N
ATOM   7573  NH2 ARG B 194      62.389  15.804  67.601  1.00 27.37           N
ANISOU 7573  NH2 ARG B 194     3325   3587   3486     89   -120     73       N
ATOM   7576  C   ARG B 194      57.203  19.345  71.396  1.00 22.88           C
ANISOU 7576  C   ARG B 194     2907   2897   2887      7     -6    -14       C
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ATOM   7577  O   ARG B 194      57.234  20.435  71.913  1.00 23.57           O
ANISOU 7577  O   ARG B 194    3005   2976   2974     54     26    -34       O
ATOM   7578  N   GLY B 195      56.058  18.788  71.086  1.00 20.97           N
ANISOU 7578  N   GLY B 195    2695   2630   2642     73     17     64       N
ATOM   7580  CA  GLY B 195      54.792  19.484  71.270  1.00 20.22           C
ANISOU 7580  CA  GLY B 195    2630   2569   2484     36    105     46       C
ATOM   7583  C   GLY B 195      54.392  20.377  70.099  1.00 18.88           C
ANISOU 7583  C   GLY B 195    2422   2417   2332    138     59     -8       C
ATOM   7584  O   GLY B 195      53.606  21.319  70.264  1.00 20.12           O
ANISOU 7584  O   GLY B 195    2613   2666   2364    157    246    -57       O
ATOM   7585  N   GLU B 196      54.940  20.122  68.914  1.00 16.10           N
ANISOU 7585  N   GLU B 196    2099   2042   1973    118     52     42       N
ATOM   7587  CA  GLU B 196      54.616  20.910  67.741  1.00 14.77           C
ANISOU 7587  CA  GLU B 196    1898   1860   1852     52     35    -23       C
ATOM   7589  CB  GLU B 196      55.843  21.648  67.191  1.00 14.83           C
ANISOU 7589  CB  GLU B 196    1880   1821   1934     56     45      4       C
ATOM   7592  CG  GLU B 196      56.669  22.388  68.189  1.00 19.90           C
ANISOU 7592  CG  GLU B 196    2487   2571   2499     24   -103     77       C
ATOM   7595  CD  GLU B 196      56.042  23.677  68.595  1.00 25.07           C
ANISOU 7595  CD  GLU B 196    3348   2966   3209    119     21   -124       C
ATOM   7596  OE1 GLU B 196      55.371  24.369  67.759  1.00 25.27           O
ANISOU 7596  OE1 GLU B 196    3342   2931   3326    147     64     59       O
ATOM   7597  OE2 GLU B 196      56.216  23.981  69.772  1.00 31.30           O
ANISOU 7597  OE2 GLU B 196    4387   3910   3594     39   -188     43       O
ATOM   7598  C   GLU B 196      54.162  20.063  66.576  1.00 12.42           C
ANISOU 7598  C   GLU B 196    1683   1560   1473     -3     71     39       C
ATOM   7599  O   GLU B 196      54.545  18.886  66.439  1.00 13.86           O
ANISOU 7599  O   GLU B 196    2002   1857   1407    240     15    111       O
ATOM   7600  N   LEU B 197      53.391  20.702  65.726  1.00  9.67           N
ANISOU 7600  N   LEU B 197    1144   1146   1384     34    104      4       N
ATOM   7602  CA  LEU B 197      53.060  20.208  64.403  1.00 10.48           C
ANISOU 7602  CA  LEU B 197    1328   1283   1369     63     16     40       C
ATOM   7604  CB  LEU B 197      51.748  20.792  63.940  1.00 11.54           C
ANISOU 7604  CB  LEU B 197    1395   1455   1533     61     74    157       C
ATOM   7607  CG  LEU B 197      50.648  20.478  64.942  1.00 16.47           C
ANISOU 7607  CG  LEU B 197    2208   2160   1890     58    123    -15       C
ATOM   7609  CD1 LEU B 197      49.393  21.367  64.753  1.00 19.37           C
ANISOU 7609  CD1 LEU B 197    2276   2531   2549     68    -62    -62       C
ATOM   7613  CD2 LEU B 197      50.295  18.970  64.876  1.00 17.62           C
ANISOU 7613  CD2 LEU B 197    2385   2132   2175   -149    187     94       C
ATOM   7617  C   LEU B 197      54.192  20.610  63.465  1.00  9.52           C
ANISOU 7617  C   LEU B 197    1237   1222   1156    131     25     75       C
ATOM   7618  O   LEU B 197      54.329  21.789  63.089  1.00  8.44           O
ANISOU 7618  O   LEU B 197    969   1215   1022    118    165     10       O
ATOM   7619  N   GLU B 198      55.050  19.628  63.166  1.00 10.81           N
ANISOU 7619  N   GLU B 198    1525   1299   1283     96    112    112       N
ATOM   7621  CA  GLU B 198      56.340  19.832  62.524  1.00 10.00           C
ANISOU 7621  CA  GLU B 198    1220   1247   1332     90    -30     -9       C
ATOM   7623  CB  GLU B 198      57.316  18.708  62.964  1.00 11.34           C
ANISOU 7623  CB  GLU B 198    1377   1460   1470     87     60     37       C
ATOM   7626  CG  GLU B 198      57.437  18.462  64.458  1.00 12.25           C
ANISOU 7626  CG  GLU B 198    1430   1534   1688    199   -126     37       C
ATOM   7629  CD  GLU B 198      58.392  19.393  65.172  1.00 15.83           C
ANISOU 7629  CD  GLU B 198    1906   1996   2110     55    -95     26       C
ATOM   7630  OE1 GLU B 198      58.756  20.454  64.601  1.00 15.70           O
ANISOU 7630  OE1 GLU B 198    1945   2094   1925     70    119    269       O
ATOM   7631  OE2 GLU B 198      58.728  19.057  66.351  1.00 15.42           O
ANISOU 7631  OE2 GLU B 198    1714   2197   1949    434    -74     85       O
ATOM   7632  C   GLU B 198      56.364  19.910  60.996  1.00  8.74           C
ANISOU 7632  C   GLU B 198    1028   1124   1168     89     13     94       C
ATOM   7633  O   GLU B 198      55.772  19.043  60.264  1.00  8.91           O
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ANISOU 7633  O   GLU B 198      880   1247   1255    144     44     82       O
ATOM   7634  N   ILE B 199     57.142  20.865  60.491  1.00  8.42           N
ANISOU 7634  N   ILE B 199     1074   1019   1106     29   -219      0       N
ATOM   7636  CA  ILE B 199     57.311  20.958  59.030  1.00  8.38           C
ANISOU 7636  CA  ILE B 199     1055   1031   1097    -48     54     47       C
ATOM   7638  CB  ILE B 199     58.004  22.290  58.569  1.00  8.06           C
ANISOU 7638  CB  ILE B 199     1021    947   1091     80    -59     34       C
ATOM   7640  CG1 ILE B 199     57.705  22.548  57.084  1.00  7.42           C
ANISOU 7640  CG1 ILE B 199      895    992    931   -143     35     31       C
ATOM   7643  CD1 ILE B 199     56.264  22.818  56.845  1.00  9.09           C
ANISOU 7643  CD1 ILE B 199     1284   1148   1019    233    -24     44       C
ATOM   7647  CG2 ILE B 199     59.536  22.259  58.748  1.00  9.61           C
ANISOU 7647  CG2 ILE B 199     1023   1095   1531   -125    -15     53       C
ATOM   7651  C   ILE B 199     58.105  19.735  58.593  1.00  8.98           C
ANISOU 7651  C   ILE B 199     1194   1130   1087     25    -70     26       C
ATOM   7652  O   ILE B 199     57.955  19.231  57.520  1.00  9.05           O
ANISOU 7652  O   ILE B 199     1443   1006    989    103   -139     85       O
ATOM   7653  N   THR B 200     58.956  19.233  59.468  1.00  9.37           N
ANISOU 7653  N   THR B 200     1308   1232   1017    123    -82     13       N
ATOM   7655  CA  THR B 200     59.813  18.165  59.104  1.00 10.32           C
ANISOU 7655  CA  THR B 200     1351   1404   1164     38    -16     35       C
ATOM   7657  CB  THR B 200     60.865  18.013  60.206  1.00  9.50           C
ANISOU 7657  CB  THR B 200     1192   1346   1071    108   -103    -54       C
ATOM   7659  OG1 THR B 200     61.743  19.168  60.167  1.00 10.06           O
ANISOU 7659  OG1 THR B 200     1261   1636    926    279    -26    -46       O
ATOM   7661  CG2 THR B 200     61.774  16.795  60.006  1.00 13.50           C
ANISOU 7661  CG2 THR B 200     1722   1822   1584    108    -69   -158       C
ATOM   7665  C   THR B 200     58.946  16.926  58.876  1.00  9.17           C
ANISOU 7665  C   THR B 200     1248   1188   1045     21     35     92       C
ATOM   7666  O   THR B 200     59.226  16.135  58.012  1.00  9.46           O
ANISOU 7666  O   THR B 200     1201   1233   1158     71    204    311       O
ATOM   7667  N   ASP B 201     57.834  16.806  59.588  1.00  8.36           N
ANISOU 7667  N   ASP B 201     1033   1105   1038    124     41    149       N
ATOM   7669  CA  ASP B 201     56.974  15.661  59.413  1.00  9.10           C
ANISOU 7669  CA  ASP B 201     1124   1242   1090    119     88    -29       C
ATOM   7671  CB  ASP B 201     55.925  15.556  60.522  1.00  9.39           C
ANISOU 7671  CB  ASP B 201     1066   1240   1260    -63    172    178       C
ATOM   7674  CG  ASP B 201     56.477  15.093  61.867  1.00 12.60           C
ANISOU 7674  CG  ASP B 201     1400   1909   1477    -34     -2     91       C
ATOM   7675  OD1 ASP B 201     57.668  14.661  61.985  1.00 14.53           O
ANISOU 7675  OD1 ASP B 201     1823   2155   1541    197    134   -158       O
ATOM   7676  OD2 ASP B 201     55.703  15.025  62.884  1.00 15.41           O
ANISOU 7676  OD2 ASP B 201     2349   1932   1572    365    174     10       O
ATOM   7677  C   ASP B 201     56.260  15.824  58.078  1.00  8.87           C
ANISOU 7677  C   ASP B 201     993   1218   1157     81     91     59       C
ATOM   7678  O   ASP B 201     55.957  14.832  57.401  1.00  8.40           O
ANISOU 7678  O   ASP B 201     940   1123   1126     99    267    114       O
ATOM   7679  N   VAL B 202     55.922  17.066  57.724  1.00  8.76           N
ANISOU 7679  N   VAL B 202     1072   1119   1135     34     24     15       N
ATOM   7681  CA  VAL B 202     55.333  17.301  56.397  1.00  9.57           C
ANISOU 7681  CA  VAL B 202     1250   1173   1212     23     11     43       C
ATOM   7683  CB  VAL B 202     55.047  18.801  56.148  1.00  9.03           C
ANISOU 7683  CB  VAL B 202     1197   1134   1097     12    -21     10       C
ATOM   7685  CG1 VAL B 202     54.641  19.053  54.692  1.00  9.40           C
ANISOU 7685  CG1 VAL B 202     1040   1250   1280   -102     27     36       C
ATOM   7689  CG2 VAL B 202     53.990  19.293  57.092  1.00  9.82           C
ANISOU 7689  CG2 VAL B 202     1239   1238   1250    194    -51     73       C
ATOM   7693  C   VAL B 202     56.297  16.810  55.316  1.00  9.16           C
ANISOU 7693  C   VAL B 202     1101   1159   1217     59     20     23       C
ATOM   7694  O   VAL B 202     55.938  16.072  54.366  1.00  7.77           O
ANISOU 7694  O   VAL B 202      891    894   1165    186    205    -26       O
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ATOM   7695  N   ASN B 203      57.525  17.287  55.426  1.00 10.20           N
ANISOU 7695  N   ASN B 203    1302   1239   1333     64     14     -4        N
ATOM   7697  CA  ASN B 203      58.559  16.932  54.459  1.00 10.05           C
ANISOU 7697  CA  ASN B 203    1273   1280   1265     10     44     32        C
ATOM   7699  CB  ASN B 203      59.814  17.761  54.717  1.00 10.06           C
ANISOU 7699  CB  ASN B 203    1169   1280   1374    111    -23    -38        C
ATOM   7702  CG  ASN B 203      59.591  19.248  54.475  1.00  9.17           C
ANISOU 7702  CG  ASN B 203    1014   1298   1171     30    140    104        C
ATOM   7703  OD1 ASN B 203      58.694  19.637  53.713  1.00  9.46           O
ANISOU 7703  OD1 ASN B 203    1124    931   1536     66    150    653        O
ATOM   7704  ND2 ASN B 203      60.311  20.072  55.210  1.00  9.01           N
ANISOU 7704  ND2 ASN B 203    1000   1014   1408     70    245    288        N
ATOM   7707  C   ASN B 203      58.824  15.410  54.397  1.00 10.07           C
ANISOU 7707  C   ASN B 203    1267   1271   1287     66     57     33        C
ATOM   7708  O   ASN B 203      59.045  14.835  53.304  1.00  9.53           O
ANISOU 7708  O   ASN B 203    1488    915   1217    -72   -123    -25        O
ATOM   7709  N   ARG B 204      58.714  14.732  55.533  1.00 10.01           N
ANISOU 7709  N   ARG B 204    1312   1309   1180     35    -10     59        N
ATOM   7711  CA  ARG B 204      58.923  13.268  55.555  1.00 10.11           C
ANISOU 7711  CA  ARG B 204    1265   1314   1259     70     48    -37        C
ATOM   7713  CB  ARG B 204      58.977  12.709  56.936  1.00 11.25           C
ANISOU 7713  CB  ARG B 204    1473   1394   1406     98    -75    -10        C
ATOM   7716  CG  ARG B 204      59.583  11.276  56.991  1.00 14.37           C
ANISOU 7716  CG  ARG B 204    2004   1721   1736    124    -69      2        C
ATOM   7719  CD  ARG B 204      59.765  10.779  58.410  1.00 14.47           C
ANISOU 7719  CD  ARG B 204    1880   1818   1799     12     -1     45        C
ATOM   7722  NE  ARG B 204      60.674  11.630  59.176  1.00 12.17           N
ANISOU 7722  NE  ARG B 204    1179   1653   1788    -15    109    109        N
ATOM   7724  CZ  ARG B 204      60.301  12.484  60.095  1.00 11.97           C
ANISOU 7724  CZ  ARG B 204    1438   1628   1479    -95     67     86        C
ATOM   7725  NH1 ARG B 204      59.017  12.602  60.429  1.00 12.86           N
ANISOU 7725  NH1 ARG B 204    1369   1644   1870     71     58   -102        N
ATOM   7728  NH2 ARG B 204      61.193  13.185  60.741  1.00 12.50           N
ANISOU 7728  NH2 ARG B 204    1488   1615   1645   -257    213    229        N
ATOM   7731  C   ARG B 204      57.807  12.534  54.827  1.00  9.34           C
ANISOU 7731  C   ARG B 204    1158   1284   1105     58     31     51        C
ATOM   7732  O   ARG B 204      58.044  11.532  54.188  1.00  8.66           O
ANISOU 7732  O   ARG B 204    812   1232   1246     19   -159     79        O
ATOM   7733  N   ALA B 205      56.596  13.095  54.872  1.00  8.96           N
ANISOU 7733  N   ALA B 205    1110   1348    944    113     34     37        N
ATOM   7735  CA  ALA B 205      55.483  12.514  54.168  1.00  9.38           C
ANISOU 7735  CA  ALA B 205    1208   1133   1221     40     42     42        C
ATOM   7737  CB  ALA B 205      54.142  13.182  54.587  1.00  9.65           C
ANISOU 7737  CB  ALA B 205    1331   1203   1132    124     16    -13        C
ATOM   7741  C   ALA B 205      55.717  12.586  52.665  1.00  9.54           C
ANISOU 7741  C   ALA B 205    1218   1185   1222     82    -41     18        C
ATOM   7743  N   TYR B 206      56.213  13.729  52.185  1.00  8.59           N
ANISOU 7743  N   TYR B 206    1099   1071   1090     67     58    -39        N
ATOM   7745  CA  TYR B 206      56.653  13.830  50.783  1.00  8.50           C
ANISOU 7745  CA  TYR B 206    1014   1125   1088     91   -101     65        C
ATOM   7747  CB  TYR B 206      57.045  15.246  50.528  1.00  7.20           C
ANISOU 7747  CB  TYR B 206     878    926    930    192    -77    -35        C
ATOM   7750  CG  TYR B 206      55.839  16.176  50.139  1.00  7.95           C
ANISOU 7750  CG  TYR B 206     748   1088   1184      9    -74    133        C
ATOM   7751  CD1 TYR B 206      55.285  17.033  51.071  1.00  5.99           C
ANISOU 7751  CD1 TYR B 206     628    728    921   -102    -74    154        C
ATOM   7753  CE1 TYR B 206      54.216  17.899  50.746  1.00  7.13           C
ANISOU 7753  CE1 TYR B 206     996    855    858     28     69    -43        C
ATOM   7762  C   TYR B 206      57.821  12.875  50.421  1.00  8.12           C
ANISOU 7762  C   TYR B 206    1099    910   1075    -23     24     44        C
ATOM   7764  N   LEU B 207      58.781  12.777  51.307  1.00  7.46           N
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ANISOU 7764  N   LEU B 207      994    765   1072    -66     23     93       N
ATOM   7766  CA  LEU B 207     59.949  11.942  51.047  1.00  9.84           C
ANISOU 7766  CA  LEU B 207     1348   1125   1264    -20    -20     22       C
ATOM   7768  CB  LEU B 207     60.944  12.060  52.198  1.00  9.38           C
ANISOU 7768  CB  LEU B 207     1252   1127   1185    -92      6     14       C
ATOM   7771  CG  LEU B 207     62.252  11.247  52.119  1.00 11.73           C
ANISOU 7771  CG  LEU B 207     1481   1539   1434     23      0     65       C
ATOM   7773  CD1 LEU B 207     63.058  11.655  50.933  1.00 12.98           C
ANISOU 7773  CD1 LEU B 207     1434   1828   1668    119    -11    174       C
ATOM   7777  CD2 LEU B 207     63.086  11.353  53.387  1.00 13.39           C
ANISOU 7777  CD2 LEU B 207     1517   1725   1844    -78    -98     47       C
ATOM   7848  CA  LEU B 212     60.552  15.519  48.012  1.00  7.58           C
ANISOU 7848  CA  LEU B 212      951    952    975     80     57     56       C
ATOM   7850  CB  LEU B 212     60.977  15.250  49.440  1.00  8.80           C
ANISOU 7850  CB  LEU B 212     1126   1076   1139    127    -59     63       C
ATOM   7853  CG  LEU B 212     61.711  16.320  50.217  1.00  8.98           C
ANISOU 7853  CG  LEU B 212     1254   1088   1070     -1    -47     93       C
ATOM   7855  CD1 LEU B 212     60.861  17.534  50.455  1.00  8.85           C
ANISOU 7855  CD1 LEU B 212      954   1309   1097    -37     24    -51       C
ATOM   7859  CD2 LEU B 212     62.288  15.776  51.576  1.00 10.09           C
ANISOU 7859  CD2 LEU B 212      943   1628   1262     51    -25    129       C
ATOM   7863  C   LEU B 212     61.815  15.786  47.229  1.00  7.10           C
ANISOU 7863  C   LEU B 212      766    895   1034     18    -23     24       C
ATOM   7865  N   SER B 213     61.913  16.976  46.696  1.00  7.08           N
ANISOU 7865  N   SER B 213      674    925   1090    -11    -47    -55       N
ATOM   7874  C   SER B 213     63.971  18.198  47.116  1.00  7.04           C
ANISOU 7874  C   SER B 213      877   1011    787     23    -55    -22       C
ATOM   7875  O   SER B 213     63.527  19.266  47.564  1.00  8.08           O
ANISOU 7875  O   SER B 213     1033   1179    858    -38      4   -193       O
ATOM   7876  N   VAL B 214     65.176  17.725  47.420  1.00  7.32           N
ANISOU 7876  N   VAL B 214      907    960    914    -22     27    -86       N
ATOM   7878  CA  VAL B 214     66.065  18.412  48.332  1.00  8.50           C
ANISOU 7878  CA  VAL B 214      992   1117   1118     26    -31      7       C
ATOM   7880  CB  VAL B 214     66.662  17.473  49.325  1.00  9.49           C
ANISOU 7880  CB  VAL B 214     1135   1234   1236    -41    -99     20       C
ATOM   7882  CG1 VAL B 214     67.640  18.265  50.220  1.00  9.17           C
ANISOU 7882  CG1 VAL B 214     1216   1187   1081    158   -197     -2       C
ATOM   7886  CG2 VAL B 214     65.557  16.808  50.137  1.00 11.30           C
ANISOU 7886  CG2 VAL B 214     1389   1327   1576     58    -56    153       C
ATOM   7890  C   VAL B 214     67.181  18.986  47.493  1.00  8.26           C
ANISOU 7890  C   VAL B 214      916   1055   1164    -59    -44     -4       C
ATOM   7891  O   VAL B 214     67.989  18.241  46.905  1.00  9.17           O
ANISOU 7891  O   VAL B 214      800   1215   1469    -74    237     171       O
ATOM   7892  N   GLU B 215     67.172  20.293  47.357  1.00  8.23           N
ANISOU 7892  N   GLU B 215      917   1057   1150     26   -148     -24       N
ATOM   7894  CA  GLU B 215     68.211  20.975  46.602  1.00  9.54           C
ANISOU 7894  CA  GLU B 215     1134   1246   1244      5      1      10       C
ATOM   7896  CB  GLU B 215     67.662  22.184  45.830  1.00 10.10           C
ANISOU 7896  CB  GLU B 215     1238   1336   1261   -114    -15      54       C
ATOM   7905  C   GLU B 215     69.311  21.454  47.534  1.00 10.31           C
ANISOU 7905  C   GLU B 215     1285   1363   1268    -32     -7      35       C
ATOM   7906  O   GLU B 215     69.015  21.990  48.613  1.00 10.95           O
ANISOU 7906  O   GLU B 215     1164   1485   1511     -3     42    -262       O
ATOM   7907  N   ILE B 216     70.582  21.269  47.143  1.00  8.84           N
ANISOU 7907  N   ILE B 216     1186   1120   1050     17    136     -41       N
ATOM   7909  CA  ILE B 216     71.663  21.828  47.943  1.00  9.55           C
ANISOU 7909  CA  ILE B 216     1186   1120   1323    -38     53     154       C
ATOM   7911  CB  ILE B 216     73.019  21.179  47.676  1.00  9.77           C
ANISOU 7911  CB  ILE B 216     1333    987   1390   -102     84      95       C
ATOM   7916  CD1 ILE B 216     72.520  19.201  49.103  1.00 12.05           C
ANISOU 7916  CD1 ILE B 216     1598   1323   1658     92    147      24       C
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ATOM   7920  CG2 ILE B 216      74.070  21.754  48.722  1.00 13.23           C
ANISOU 7920  CG2 ILE B 216    1725   1640   1660     77    -40     68       C
ATOM   7924  C   ILE B 216      71.764  23.376  47.628  1.00  9.10           C
ANISOU 7924  C   ILE B 216    1022   1150   1284    -74     58     42       C
ATOM   7926  N   MET B 217      71.750  24.157  48.702  1.00  7.68           N
ANISOU 7926  N   MET B 217     609   1083   1225    -68     47     -9       N
ATOM   7928  CA  MET B 217      72.067  25.557  48.649  1.00  8.58           C
ANISOU 7928  CA  MET B 217     947   1130   1180    -11    -66     39       C
ATOM   7930  CB  MET B 217      71.215  26.316  49.614  1.00  9.01           C
ANISOU 7930  CB  MET B 217    1087   1149   1187    -42    -41    -31       C
ATOM   7933  CG  MET B 217      71.532  27.850  49.786  1.00 10.49           C
ANISOU 7933  CG  MET B 217    1444   1082   1457    -75    -43    172       C
ATOM   7936  SD  MET B 217      70.285  28.672  50.856  1.00 12.06           S
ANISOU 7936  SD  MET B 217    1553   1472   1554    196     -5    -92       S
ATOM   7937  CE  MET B 217      68.809  28.514  49.872  1.00 13.78           C
ANISOU 7937  CE  MET B 217    1799   1689   1747    -59    188    138       C
ATOM   7941  C   MET B 217      73.554  25.671  49.012  1.00  7.98           C
ANISOU 7941  C   MET B 217     960    984   1088     -4    -22    -25       C
ATOM   7942  O   MET B 217      73.983  25.471  50.156  1.00  9.87           O
ANISOU 7942  O   MET B 217    1136   1378   1233     46    -49     97       O
ATOM   7985  CB  TYR B 221      73.672  30.854  49.426  1.00  7.23           C
ANISOU 7985  CB  TYR B 221     960    899    887     60    -74     86       C
ATOM   8000  C   TYR B 221      75.110  31.869  51.094  1.00  8.55           C
ANISOU 8000  C   TYR B 221    1222   1053    971     35    -17    -38       C
ATOM   8001  O   TYR B 221      75.737  31.045  51.754  1.00  9.15           O
ANISOU 8001  O   TYR B 221    1659   1026    790    301   -188   -143       O
ATOM   8002  N   ALA B 222      74.590  32.977  51.612  1.00  8.75           N
ANISOU 8002  N   ALA B 222    1042   1052   1230    134     29    102       N
ATOM   8004  CA  ALA B 222      74.490  33.151  53.032  1.00  9.59           C
ANISOU 8004  CA  ALA B 222    1092   1207   1344     87     -1     51       C
ATOM   8006  CB  ALA B 222      74.801  34.548  53.454  1.00 11.40           C
ANISOU 8006  CB  ALA B 222    1295   1475   1559    -94    103    -38       C
ATOM   8010  C   ALA B 222      73.055  32.801  53.417  1.00 10.24           C
ANISOU 8010  C   ALA B 222    1158   1337   1395    -75     98    121       C
ATOM   8011  O   ALA B 222      72.111  33.257  52.772  1.00  8.71           O
ANISOU 8011  O   ALA B 222     748   1108   1453   -277    191    100       O
ATOM   8012  N   TRP B 223      72.927  31.966  54.433  1.00 10.57           N
ANISOU 8012  N   TRP B 223    1245   1424   1345     17     81     91       N
ATOM   8014  CA  TRP B 223      71.617  31.648  55.060  1.00  9.73           C
ANISOU 8014  CA  TRP B 223    1096   1348   1250    -25     -9     12       C
ATOM   8016  CB  TRP B 223      71.184  30.192  54.891  1.00 10.75           C
ANISOU 8016  CB  TRP B 223    1287   1554   1243    -72     26     34       C
ATOM   8019  CG  TRP B 223      69.899  29.871  55.706  1.00  8.42           C
ANISOU 8019  CG  TRP B 223     965   1209   1024   -108    -24   -124       C
ATOM   8020  CD1 TRP B 223      68.777  30.564  55.722  1.00 11.01           C
ANISOU 8020  CD1 TRP B 223    1576   1392   1216    -25    -62     78       C
ATOM   8022  NE1 TRP B 223      67.868  30.014  56.604  1.00 10.77           N
ANISOU 8022  NE1 TRP B 223    1066   1479   1544    -85    238     46       N
ATOM   8024  CE2 TRP B 223      68.482  28.978  57.262  1.00  9.41           C
ANISOU 8024  CE2 TRP B 223    1173   1284   1116     88    205     -33       C
ATOM   8025  CD2 TRP B 223      69.753  28.847  56.705  1.00 10.61           C
ANISOU 8025  CD2 TRP B 223    1055   1431   1545   -103     35      2       C
ATOM   8026  CE3 TRP B 223      70.584  27.825  57.182  1.00 10.23           C
ANISOU 8026  CE3 TRP B 223    1311   1107   1466    -59    -10     144       C
ATOM   8028  CZ3 TRP B 223      70.117  26.979  58.160  1.00  9.84           C
ANISOU 8028  CZ3 TRP B 223    1148   1407   1182     45     95     -61       C
ATOM   8030  CH2 TRP B 223      68.855  27.118  58.669  1.00  8.97           C
ANISOU 8030  CH2 TRP B 223     956   1151   1300    -287    314     189       C
ATOM   8032  CZ2 TRP B 223      68.006  28.095  58.219  1.00  9.05           C
ANISOU 8032  CZ2 TRP B 223    1018   1072   1348    -71     74     -65       C
ATOM   8034  C   TRP B 223      71.869  31.908  56.530  1.00 12.21           C
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ANISOU 8034  C   TRP B 223     1507   1706   1426     23    106    131       C
ATOM   8035  O   TRP B 223      72.679  31.207  57.206  1.00 12.56           O
ANISOU 8035  O   TRP B 223     1512   1769   1490    191    130    164       O
ATOM   8036  N   LEU B 224      71.202  32.910  57.044  1.00 13.37           N
ANISOU 8036  N   LEU B 224     1845   1630   1605    125     -8     85       N
ATOM   8038  CA  LEU B 224      71.365  33.268  58.431  1.00 16.15           C
ANISOU 8038  CA  LEU B 224     2148   1939   2046     20    -24    -15       C
ATOM   8040  CB  LEU B 224      71.968  34.652  58.499  1.00 15.97           C
ANISOU 8040  CB  LEU B 224     2147   1959   1960      3    -41     62       C
ATOM   8043  CG  LEU B 224      73.181  34.812  57.629  1.00 16.95           C
ANISOU 8043  CG  LEU B 224     2208   2006   2223    -30    -11    -31       C
ATOM   8045  CD1 LEU B 224      73.511  36.294  57.545  1.00 17.91           C
ANISOU 8045  CD1 LEU B 224     2639   2042   2123   -104     95    -78       C
ATOM   8049  CD2 LEU B 224      74.332  33.994  58.192  1.00 16.82           C
ANISOU 8049  CD2 LEU B 224     2057   2028   2304    -97    -33    -44       C
ATOM   8053  C   LEU B 224      70.001  33.280  59.080  1.00 17.40           C
ANISOU 8053  C   LEU B 224     2296   2140   2172     -5     24     11       C
ATOM   8054  O   LEU B 224      68.990  33.461  58.434  1.00 17.58           O
ANISOU 8054  O   LEU B 224     2358   2193   2125    -82    128     51       O
ATOM   8055  N   ASP B 225      69.972  33.108  60.384  1.00 20.27           N
ANISOU 8055  N   ASP B 225     2661   2523   2518    -43     22    -61       N
ATOM   8057  CA  ASP B 225      68.730  33.298  61.076  1.00 21.74           C
ANISOU 8057  CA  ASP B 225     2821   2776   2662     -5     -8    -70       C
ATOM   8059  CB  ASP B 225      68.103  31.958  61.370  1.00 24.35           C
ANISOU 8059  CB  ASP B 225     3126   3088   3038   -132     73    -32       C
ATOM   8062  CG  ASP B 225      68.286  31.510  62.753  1.00 27.20           C
ANISOU 8062  CG  ASP B 225     3643   3475   3213    -41   -155     58       C
ATOM   8063  OD1 ASP B 225      67.837  32.209  63.661  1.00 28.91           O
ANISOU 8063  OD1 ASP B 225     4029   3334   3622     57    179     16       O
ATOM   8064  OD2 ASP B 225      68.776  30.406  62.998  1.00 35.41           O
ANISOU 8064  OD2 ASP B 225     4537   4026   4890    256   -187    -74       O
ATOM   8065  C   ASP B 225      68.953  34.252  62.271  1.00 20.97           C
ANISOU 8065  C   ASP B 225     2675   2670   2623    -20     25    -96       C
ATOM   8066  O   ASP B 225      69.994  34.295  62.892  1.00 19.64           O
ANISOU 8066  O   ASP B 225     2782   2562   2117     99     -4   -326       O
ATOM   8067  N   THR B 226      67.989  35.112  62.462  1.00 21.71           N
ANISOU 8067  N   THR B 226     2736   2756   2757    -64    -22    -61       N
ATOM   8069  CA  THR B 226      68.089  36.091  63.502  1.00 22.49           C
ANISOU 8069  CA  THR B 226     2811   2826   2905    -36     -3    -27       C
ATOM   8071  CB  THR B 226      67.423  37.337  63.054  1.00 23.27           C
ANISOU 8071  CB  THR B 226     2843   2945   3053    -12    -38      9       C
ATOM   8073  OG1 THR B 226      65.995  37.123  63.017  1.00 25.90           O
ANISOU 8073  OG1 THR B 226     2876   3306   3656   -164     94    193       O
ATOM   8075  CG2 THR B 226      67.810  37.653  61.618  1.00 22.07           C
ANISOU 8075  CG2 THR B 226     2778   2765   2841    -22    -10    -42       C
ATOM   8079  C   THR B 226      67.500  35.666  64.814  1.00 22.74           C
ANISOU 8079  C   THR B 226     2777   2881   2981    -44     46      5       C
ATOM   8080  O   THR B 226      67.089  36.498  65.584  1.00 23.28           O
ANISOU 8080  O   THR B 226     2840   2889   3116    -69    102     16       O
ATOM   8081  N   GLY B 227      67.607  34.401  65.160  1.00 23.41           N
ANISOU 8081  N   GLY B 227     3006   2911   2978   -153     91    -18       N
ATOM   8083  CA  GLY B 227      67.015  33.944  66.426  1.00 23.57           C
ANISOU 8083  CA  GLY B 227     3046   2993   2915    -78     19    -36       C
ATOM   8086  C   GLY B 227      67.648  34.275  67.769  1.00 22.92           C
ANISOU 8086  C   GLY B 227     3004   2895   2808    -46    133    -59       C
ATOM   8087  O   GLY B 227      66.902  34.104  68.749  1.00 23.27           O
ANISOU 8087  O   GLY B 227     3199   2856   2787   -100    309   -211       O
ATOM   8088  N   THR B 228      68.974  34.570  67.831  1.00 19.39           N
ANISOU 8088  N   THR B 228     2837   2456   2419   -190    118    -77       N
ATOM   8090  CA  THR B 228      69.693  34.910  69.038  1.00 19.39           C
ANISOU 8090  CA  THR B 228     2617   2246   2501   -142     75     58       C
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ATOM   8092  CB  THR B 228      70.895  34.051  69.304  1.00 19.57           C
ANISOU 8092  CB  THR B 228    2629   2279   2527    -94     91    -61       C
ATOM   8094  OG1 THR B 228      71.812  34.144  68.199  1.00 21.77           O
ANISOU 8094  OG1 THR B 228    3277   2154   2841   -117    367     50       O
ATOM   8096  CG2 THR B 228      70.526  32.524  69.512  1.00 20.69           C
ANISOU 8096  CG2 THR B 228    2719   2534   2608   -101     76     90       C
ATOM   8100  C   THR B 228      70.188  36.343  68.959  1.00 17.65           C
ANISOU 8100  C   THR B 228    2403   2118   2185   -176     -1    -26       C
ATOM   8101  O   THR B 228      70.216  36.958  67.898  1.00 15.76           O
ANISOU 8101  O   THR B 228    2356   1620   2009   -393    -14     76       O
ATOM   8102  N   HIS B 229      70.563  36.882  70.104  1.00 16.06           N
ANISOU 8102  N   HIS B 229    2218   1857   2024   -167     23      8       N
ATOM   8104  CA  HIS B 229      71.014  38.257  70.095  1.00 14.52           C
ANISOU 8104  CA  HIS B 229    1963   1683   1870    -48    -14    -29       C
ATOM   8106  CB  HIS B 229      71.367  38.720  71.493  1.00 12.98           C
ANISOU 8106  CB  HIS B 229    1851   1417   1661   -165     -8   -107       C
ATOM   8109  CG  HIS B 229      70.228  38.719  72.432  1.00 10.75           C
ANISOU 8109  CG  HIS B 229    1570    998   1515   -106   -125   -118       C
ATOM   8110  ND1 HIS B 229      70.306  38.140  73.687  1.00 12.38           N
ANISOU 8110  ND1 HIS B 229    1719   1435   1551    141    121   -129       N
ATOM   8112  CE1 HIS B 229      69.188  38.392  74.341  1.00 13.36           C
ANISOU 8112  CE1 HIS B 229    1596   1672   1807     -1     58     52       C
ATOM   8114  NE2 HIS B 229      68.403  39.115  73.561  1.00 11.34           N
ANISOU 8114  NE2 HIS B 229    1629   1145   1532    -24    -25    -34       N
ATOM   8116  CD2 HIS B 229      68.985  39.232  72.329  1.00 10.57           C
ANISOU 8116  CD2 HIS B 229    1711    980   1322   -127    -33    -94       C
ATOM   8118  C   HIS B 229      72.231  38.368  69.260  1.00 13.81           C
ANISOU 8118  C   HIS B 229    1919   1611   1714    -12     66    -69       C
ATOM   8119  O   HIS B 229      72.391  39.322  68.535  1.00 13.96           O
ANISOU 8119  O   HIS B 229    2023   1474   1807     68    225   -164       O
ATOM   8120  N   ASP B 230      73.129  37.408  69.420  1.00 13.86           N
ANISOU 8120  N   ASP B 230    1791   1682   1790    -25     21     26       N
ATOM   8122  CA  ASP B 230      74.367  37.415  68.663  1.00 15.10           C
ANISOU 8122  CA  ASP B 230    1984   1860   1890    -21     38     28       C
ATOM   8124  CB  ASP B 230      75.299  36.287  69.112  1.00 15.54           C
ANISOU 8124  CB  ASP B 230    1969   1958   1978     12     44     85       C
ATOM   8130  C   ASP B 230      74.135  37.259  67.186  1.00 14.28           C
ANISOU 8130  C   ASP B 230    1804   1803   1818   -101     15      2       C
ATOM   8131  O   ASP B 230      74.811  37.912  66.392  1.00 14.14           O
ANISOU 8131  O   ASP B 230    1804   1661   1907   -126     45    122       O
ATOM   8132  N   SER B 231      73.234  36.341  65.805  1.00 14.19           N
ANISOU 8132  N   SER B 231    1809   1725   1855   -115    101     -1       N
ATOM   8134  CA  SER B 231      72.978  36.049  65.396  1.00 13.24           C
ANISOU 8134  CA  SER B 231    1611   1638   1780    -69      9      3       C
ATOM   8136  CB  SER B 231      72.173  34.683  65.203  1.00 14.74           C
ANISOU 8136  CB  SER B 231    1844   1772   1983      7    -42   -128       C
ATOM   8139  OG  SER B 231      70.734  34.754  65.306  1.00 15.47           O
ANISOU 8139  OG  SER B 231    1822   1945   2109    -76    153    -73       O
ATOM   8141  C   SER B 231      72.380  37.308  64.708  1.00 12.47           C
ANISOU 8141  C   SER B 231    1639   1431   1666    -63     70    -57       C
ATOM   8142  O   SER B 231      72.682  37.597  63.536  1.00 11.46           O
ANISOU 8142  O   SER B 231    1785    951   1618    -23    365   -156       O
ATOM   8143  N   LEU B 232      71.473  38.004  65.392  1.00 10.76           N
ANISOU 8143  N   LEU B 232    1542   1254   1292   -141     79   -144       N
ATOM   8145  CA  LEU B 232      70.833  39.173  64.828  1.00 10.71           C
ANISOU 8145  CA  LEU B 232    1301   1471   1295    -28    -12    -63       C
ATOM   8147  CB  LEU B 232      69.674  39.600  65.742  1.00 12.65           C
ANISOU 8147  CB  LEU B 232    1586   1662   1558    -31     41    -10       C
ATOM   8150  CG  LEU B 232      68.974  40.917  65.467  1.00 13.28           C
ANISOU 8150  CG  LEU B 232    1497   1844   1702    -19     55    -64       C
ATOM   8152  CD1 LEU B 232      68.267  40.897  64.154  1.00 16.56           C
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ANISOU 8152  CD1 LEU B 232     1673   2449   2168   -162     39     38       C
ATOM   8156  CD2 LEU B 232      68.084  41.261  66.676  1.00 12.73           C
ANISOU 8156  CD2 LEU B 232     1179   1800   1858    -90    -37     33       C
ATOM   8160  C   LEU B 232      71.868  40.286  64.594  1.00 11.07           C
ANISOU 8160  C   LEU B 232     1453   1408   1344    -28    -70     -4       C
ATOM   8161  O   LEU B 232      71.887  40.941  63.561  1.00  9.66           O
ANISOU 8161  O   LEU B 232     1185   1208   1275    -82    -64    -59       O
ATOM   8162  N   LEU B 233      72.812  40.429  65.515  1.00 10.93           N
ANISOU 8162  N   LEU B 233     1423   1425   1302    -80     71    -36       N
ATOM   8196  N   ALA B 235      73.908  39.354  61.533  1.00  9.24           N
ANISOU 8196  N   ALA B 235     1317   1086   1107     89    112     55       N
ATOM   8198  CA  ALA B 235      73.177  39.535  60.316  1.00 10.26           C
ANISOU 8198  CA  ALA B 235     1340   1204   1354    -31    -10    -55       C
ATOM   8200  CB  ALA B 235      71.761  39.087  60.487  1.00  9.61           C
ANISOU 8200  CB  ALA B 235     1306   1066   1276    -30     64    -27       C
ATOM  17420  O   THR D 240      79.115  33.191  59.546  1.00  9.27           O
ANISOU17420  O   THR D 240     1167   1036   1319    -98   -359   -259       O
ATOM  17467  C   ASN D 243      79.478  29.829  61.792  1.00 10.18           C
ANISOU17467  C   ASN D 243     1366   1222   1279     48     21     71       C
ATOM  17468  O   ASN D 243      79.019  28.935  62.519  1.00 10.23           O
ANISOU17468  O   ASN D 243     1155   1331   1399    225     13    377       O
ATOM  17469  N   ARG D 244      78.789  30.286  60.760  1.00  9.26           N
ANISOU17469  N   ARG D 244     1248   1121   1149     17    -22     89       N
ATOM  17471  CA  ARG D 244      77.483  29.788  60.455  1.00  9.26           C
ANISOU17471  CA  ARG D 244     1298   1041   1176      0    -27     34       C
ATOM  17473  CB  ARG D 244      76.769  30.790  59.523  1.00 10.39           C
ANISOU17473  CB  ARG D 244     1359   1239   1349     37    -78      5       C
ATOM  17476  CG  ARG D 244      75.417  30.298  58.996  1.00 11.21           C
ANISOU17476  CG  ARG D 244     1637   1282   1339     47   -103     -6       C
ATOM  17479  CD  ARG D 244      74.430  30.138  60.075  1.00 11.36           C
ANISOU17479  CD  ARG D 244     1341   1381   1595    -33     51     39       C
ATOM  17482  NE  ARG D 244      73.085  30.023  59.624  1.00  9.24           N
ANISOU17482  NE  ARG D 244     1461   1237    810    284     49   -161       N
ATOM  17484  CZ  ARG D 244      72.069  29.775  60.415  1.00 11.87           C
ANISOU17484  CZ  ARG D 244     1364   1731   1416   -199    -60    -86       C
ATOM  17485  NH1 ARG D 244      72.255  29.524  61.720  1.00 13.92           N
ANISOU17485  NH1 ARG D 244     1288   2228   1772     10    -98    315       N
ATOM  17488  NH2 ARG D 244      70.850  29.797  59.913  1.00  9.39           N
ANISOU17488  NH2 ARG D 244     909   1649   1009    210    306   -109       N
ATOM  17491  C   ARG D 244      77.586  28.425  59.761  1.00  8.39           C
ANISOU17491  C   ARG D 244     1119    991   1078     38    -63     16       C
ATOM  17492  O   ARG D 244      76.885  27.462  60.115  1.00  7.53           O
ANISOU17492  O   ARG D 244     1172    682   1004    -41     21    -26       O
ATOM  17493  N   GLN D 245      78.520  28.342  58.845  1.00  8.85           N
ANISOU17493  N   GLN D 245     1270    947   1144    -53    -41      2       N
ATOM  17495  CA  GLN D 245      78.627  27.167  57.941  1.00  9.62           C
ANISOU17495  CA  GLN D 245     1224   1151   1277    -46    -69    -52       C
ATOM  17497  CB  GLN D 245      79.170  27.564  56.609  1.00  9.49           C
ANISOU17497  CB  GLN D 245     1243   1131   1230    -66    -18    -79       C
ATOM  17500  CG  GLN D 245      78.366  28.541  55.821  1.00  9.07           C
ANISOU17500  CG  GLN D 245     841   1168   1435   -167     26      4       C
ATOM  17508  C   GLN D 245      79.464  25.976  58.437  1.00 10.04           C
ANISOU17508  C   GLN D 245     1220   1191   1401     25   -110    -43       C
ATOM  17509  O   GLN D 245      79.221  24.855  58.044  1.00  9.65           O
ANISOU17509  O   GLN D 245     1060   1283   1322     -8   -336    -52       O
ATOM  36667  O41 TDG L 500      54.446  27.838  65.670  1.00 16.05           O
ANISOU36667  O41 TDG L 500     1569   2473   2054    264    289    160       O
ATOM  36668  C41 TDG L 500      55.391  28.673  65.287  1.00 16.68           C
ANISOU36668  C41 TDG L 500     1976   2244   2117     89    323    108       C
ATOM  36669  N31 TDG L 500      55.024  29.804  64.759  1.00 14.38           N
ANISOU36669  N31 TDG L 500     1358   2321   1785    139    395     60       N
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ATOM  36671  C21 TDG L 500      55.931  30.667  64.281  1.00 15.80           C
ANISOU36671  C21 TDG L 500    1929   1930   2143    -78     10     47       C
ATOM  36672  O21 TDG L 500      55.497  31.766  63.737  1.00 14.30           O
ANISOU36672  O21 TDG L 500    1546   1580   2307   -198    326    -24       O
ATOM  36673  C51 TDG L 500      56.754  28.374  65.373  1.00 18.47           C
ANISOU36673  C51 TDG L 500    2043   2422   2551     -1     85     30       C
ATOM  36674  C5A TDG L 500      57.220  27.088  65.971  1.00 20.79           C
ANISOU36674  C5A TDG L 500    2525   2835   2538     29    176    142       C
ATOM  36678  C61 TDG L 500      57.671  29.264  64.819  1.00 17.12           C
ANISOU36678  C61 TDG L 500    1833   2125   2546     53     20     29       C
ATOM  36680  N11 TDG L 500      57.228  30.388  64.291  1.00 16.47           N
ANISOU36680  N11 TDG L 500    1862   2126   2268   -225    -34     56       N
ATOM  36681  C1, TDG L 500      58.148  31.325  63.664  1.00 18.34           C
ANISOU36681  C1, TDG L 500    2114   2433   2422     53    100    132       C
ATOM  36683  C2, TDG L 500      59.217  31.851  64.508  1.00 19.71           C
ANISOU36683  C2, TDG L 500    2420   2409   2657    -94    256   -170       C
ATOM  36686  O4, TDG L 500      58.876  30.519  62.754  1.00 18.66           O
ANISOU36686  O4, TDG L 500    2173   2250   2665    -68    -44      5       O
ATOM  36687  C4, TDG L 500      60.207  30.990  62.749  1.00 18.80           C
ANISOU36687  C4, TDG L 500    2303   2344   2494     17     88    -43       C
ATOM  36689  C3, TDG L 500      60.435  32.248  63.645  1.00 18.57           C
ANISOU36689  C3, TDG L 500    2205   2303   2548    -47    168    -42       C
ATOM  36691  O3, TDG L 500      60.258  33.249  62.659  1.00 17.42           O
ANISOU36691  O3, TDG L 500    2073   2270   2275   -297    315   -181       O
ATOM  36693  C5, TDG L 500      61.088  29.811  63.095  1.00 18.43           C
ANISOU36693  C5, TDG L 500    2244   2322   2434     98    -74   -122       C
ATOM  36696  O5, TDG L 500      60.989  29.542  64.467  1.00 22.36           O
ANISOU36696  O5, TDG L 500    2880   2881   2733    275    191   -158       O
ATOM  36697  P   TDG L 500      62.331  29.087  65.219  1.00 26.22           P
ANISOU36697  P   TDG L 500    3505   3033   3422    588    159    -35       P
ATOM  36698  O1P TDG L 500      61.807  28.579  66.646  1.00 27.82           O
ANISOU36698  O1P TDG L 500    4304   3274   2990    563   -232     83       O
ATOM  36699  O2P TDG L 500      63.615  29.855  64.751  1.00 25.15           O
ANISOU36699  O2P TDG L 500    3365   2913   3276    294   -221     62       O
ATOM  36700  OPP TDG L 500      62.717  27.816  64.322  1.00 27.90           O
ANISOU36700  OPP TDG L 500    4155   3471   2971    195   -112   -294       O
ATOM  36701  P2  TDG L 500      62.591  26.341  64.812  1.00 29.58           P
ANISOU36701  P2  TDG L 500    4200   3860   3178     -7     26   -243       P
ATOM  36702  O3P TDG L 500      61.020  26.110  64.953  1.00 29.31           O
ANISOU36702  O3P TDG L 500    3819   4136   3180    257    225    115       O
ATOM  36703  O4P TDG L 500      63.661  26.033  65.922  1.00 24.37           O
ANISOU36703  O4P TDG L 500    3580   2723   2955     18    -69   -486       O
ATOM  36704  O1  TDG L 500      63.071  25.488  63.496  1.00 19.99           O
ANISOU36704  O1  TDG L 500    3073   2037   2482    -46    -23   -123       O
ATOM  36705  C1  TDG L 500      62.328  25.527  62.258  1.00 17.60           C
ANISOU36705  C1  TDG L 500    2364   1979   2342    -69    -36     -2       C
ATOM  36707  C2  TDG L 500      62.164  24.153  61.715  1.00 13.60           C
ANISOU36707  C2  TDG L 500    1720   1793   1652     56   -136     12       C
ATOM  36709  O2  TDG L 500      61.456  23.364  62.660  1.00 13.31           O
ANISOU36709  O2  TDG L 500    1841   1856   1357    238    194   -113       O
ATOM  36711  C3  TDG L 500      63.507  23.538  61.349  1.00 12.52           C
ANISOU36711  C3  TDG L 500    1659   1829   1266     26    -45     31       C
ATOM  36713  O3  TDG L 500      63.226  22.327  60.641  1.00 12.02           O
ANISOU36713  O3  TDG L 500    1688   1740   1136   -108    516    -75       O
ATOM  36715  C4  TDG L 500      64.318  24.529  60.539  1.00 13.54           C
ANISOU36715  C4  TDG L 500    1641   1694   1809     83    -23     29       C
ATOM  36717  O4  TDG L 500      65.621  24.046  60.272  1.00 10.48           O
ANISOU36717  O4  TDG L 500    1078   1363   1541     72   -249    494       O
ATOM  36719  C5  TDG L 500      64.470  25.920  61.165  1.00 16.65           C
ANISOU36719  C5  TDG L 500    2262   2094   1969    108    102    -31       C
ATOM  36721  O5  TDG L 500      63.228  26.415  61.567  1.00 17.26           O
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ANISOU36721	O5	TDG	L	500	1951	2339	2266	-60	174	8	O
ATOM 36722	C6	TDG	L	500	64.967	26.933	60.143	1.00	15.14		C
ANISOU36722	C6	TDG	L	500	1943	1879	1928	96	78	-16	C
ATOM 36725	O6	TDG	L	500	65.056	28.265	60.654	1.00	16.12		O
ANISOU36725	O6	TDG	L	500	2163	1934	2024	171	-258	70	O
ATOM 37512	S	SO4	B	700	62.058	31.485	70.618	1.00	53.92		S
ANISOU37512	S	SO4	B	700	6820	6777	6889	-172	3	-96	S
ATOM 37513	O1	SO4	B	700	61.130	32.036	71.597	1.00	52.22		O
ANISOU37513	O1	SO4	B	700	6626	6481	6732	-73	-42	-42	O
ATOM 37514	O2	SO4	B	700	62.105	30.029	70.771	1.00	55.88		O
ANISOU37514	O2	SO4	B	700	7153	6931	7146	28	37	40	O
ATOM 37515	O3	SO4	B	700	61.531	31.799	69.278	1.00	54.98		O
ANISOU37515	O3	SO4	B	700	6988	6870	7029	-96	66	94	O
ATOM 37516	O4	SO4	B	700	63.438	31.980	70.796	1.00	53.10		O
ANISOU37516	O4	SO4	B	700	6659	6740	6777	4	47	-49	O
ATOM 37527	O5	CIT	E	1	69.575	33.835	75.731	1.00	36.63		O
ANISOU37527	O5	CIT	E	1	4868	4636	4412	-11	2	-49	O
ATOM 37528	C6	CIT	E	1	70.791	33.888	75.416	1.00	39.35		C
ANISOU37528	C6	CIT	E	1	4981	4998	4970	-12	18	23	C
ATOM 37529	O6	CIT	E	1	71.247	32.998	74.674	1.00	41.58		O
ANISOU37529	O6	CIT	E	1	5266	5111	5422	35	80	17	O
ATOM 37531	C3	CIT	E	1	71.718	34.993	75.900	1.00	39.47		C
ANISOU37531	C3	CIT	E	1	5003	5011	4981	-34	-14	-31	C
ATOM 37534	C4	CIT	E	1	72.232	35.805	74.701	1.00	39.05		C
ANISOU37534	C4	CIT	E	1	4897	5038	4900	18	-48	-36	C
ATOM 37614	O	HOH	I	18	75.994	24.384	51.895	1.00	11.33		O
ANISOU37614	O	HOH	I	18	1664	1593	1047	-215	167	-22	O
ATOM 37647	O	HOH	I	29	69.846	13.685	61.690	1.00	15.13		O
ANISOU37647	O	HOH	I	29	2063	1510	2174	128	377	-197	O
ATOM 37668	O	HOH	I	36	76.863	26.212	53.757	1.00	9.98		O
ANISOU37668	O	HOH	I	36	1199	1323	1268	-66	-33	170	O
ATOM 37680	O	HOH	I	40	64.904	35.880	53.349	1.00	17.08		O
ANISOU37680	O	HOH	I	40	2598	2067	1824	30	-347	-142	O
ATOM 37701	O	HOH	I	47	77.668	16.261	56.572	1.00	20.19		O
ANISOU37701	O	HOH	I	47	2668	2473	2530	119	84	212	O
ATOM 37719	O	HOH	I	53	47.557	27.708	67.146	1.00	18.50		O
ANISOU37719	O	HOH	I	53	2525	2302	2200	-154	134	-122	O
ATOM 37740	O	HOH	I	60	71.149	41.852	68.585	1.00	16.78		O
ANISOU37740	O	HOH	I	60	2932	2082	1359	-29	-19	-230	O
ATOM 37773	O	HOH	I	71	43.346	30.828	55.249	1.00	15.85		O
ANISOU37773	O	HOH	I	71	1508	2701	1812	82	305	-91	O
ATOM 37788	O	HOH	I	76	62.294	19.912	57.381	1.00	12.75		O
ANISOU37788	O	HOH	I	76	1448	1729	1668	-99	-37	182	O
ATOM 37803	O	HOH	I	81	68.499	13.187	59.247	1.00	13.36		O
ANISOU37803	O	HOH	I	81	1789	1385	1901	206	125	212	O
ATOM 37818	O	HOH	I	86	63.131	10.442	57.959	1.00	16.21		O
ANISOU37818	O	HOH	I	86	1655	1692	2812	-149	125	110	O
ATOM 37953	O	HOH	I	131	66.650	37.845	52.521	1.00	16.65		O
ANISOU37953	O	HOH	I	131	2378	2237	1711	285	-40	-100	O
ATOM 38043	O	HOH	I	161	70.030	10.989	65.274	1.00	24.84		O
ANISOU38043	O	HOH	I	161	3597	2513	3327	7	-365	150	O
ATOM 38052	O	HOH	I	164	63.244	22.509	57.989	1.00	11.26		O
ANISOU38052	O	HOH	I	164	1245	1879	1151	265	104	4	O
ATOM 38064	O	HOH	I	168	64.424	24.683	52.860	1.00	13.22		O
ANISOU38064	O	HOH	I	168	1669	2056	1298	113	54	-362	O
ATOM 38118	O	HOH	I	186	73.717	35.735	61.533	1.00	19.65		O
ANISOU38118	O	HOH	I	186	2692	2625	2147	-294	252	-240	O
ATOM 38148	O	HOH	I	196	53.881	16.917	63.619	1.00	16.26		O
ANISOU38148	O	HOH	I	196	1583	2145	2448	-536	140	-32	O
ATOM 38154	O	HOH	I	198	65.463	37.846	49.824	1.00	22.03		O
ANISOU38154	O	HOH	I	198	2698	2814	2858	87	-60	796	O

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ATOM  38163  O   HOH I 201      47.058  18.330  62.254  1.00 26.88           O
ANISOU38163  O   HOH I 201    3265   3527   3418     42    445    -11       O
ATOM  38334  O   HOH I 258      69.808  35.222  72.438  1.00 24.62           O
ANISOU38334  O   HOH I 258    3745   2789   2818   -409    102     51       O
ATOM  38346  O   HOH I 262      50.813  21.155  68.244  1.00 26.04           O
ANISOU38346  O   HOH I 262    3008   3367   3517    194    513    281       O
ATOM  38361  O   HOH I 267      62.711  47.610  62.362  1.00 24.59           O
ANISOU38361  O   HOH I 267    3274   2644   3422     70   -234     58       O
ATOM  38445  O   HOH I 295      53.113  32.228  66.808  1.00 20.26           O
ANISOU38445  O   HOH I 295    2166   2797   2733   -288    308   -232       O
ATOM  38499  O   HOH I 313      59.399  21.295  62.197  1.00 25.28           O
ANISOU38499  O   HOH I 313    2737   4099   2766   -583   -165    224       O
ATOM  38589  O   HOH I 343      51.022  32.526  68.454  1.00 21.81           O
ANISOU38589  O   HOH I 343    2945   2819   2521    -69    357     -9       O
ATOM  38598  O   HOH I 346      72.696  33.012  61.616  1.00 19.19           O
ANISOU38598  O   HOH I 346    2474   2770   2047   -342   -553   -264       O
ATOM  38664  O   HOH I 368      57.245  23.427  64.260  1.00 18.33           O
ANISOU38664  O   HOH I 368    1806   2443   2715    127    280    389       O
ATOM  38766  O   HOH I 402      75.227  26.990  62.330  1.00 23.67           O
ANISOU38766  O   HOH I 402    2836   3702   2453   -132   -306   -308       O
ATOM  38793  O   HOH I 411      43.770  31.241  63.622  1.00 27.56           O
ANISOU38793  O   HOH I 411    3588   3638   3244   -132    186   -444       O
ATOM  38796  O   HOH I 412      67.213  13.851  69.612  1.00 24.16           O
ANISOU38796  O   HOH I 412    2850   3149   3180   -252     87    347       O
ATOM  38802  O   HOH I 414      78.149  33.255  62.147  1.00 20.45           O
ANISOU38802  O   HOH I 414    2877   2503   2390   -204    336    229       O
ATOM  38823  O   HOH I 421      49.500  38.544  60.745  1.00 21.54           O
ANISOU38823  O   HOH I 421    2870   3024   2288    232    445    155       O
ATOM  38826  O   HOH I 422      46.316  19.931  64.291  1.00 31.72           O
ANISOU38826  O   HOH I 422    4227   4019   3804   -132    425   -152       O
ATOM  38952  O   HOH I 464      59.068  37.526  68.769  1.00 26.15           O
ANISOU38952  O   HOH I 464    3620   3246   3071   -420    179    348       O
ATOM  39012  O   HOH I 484      73.214  35.582  71.694  1.00 28.62           O
ANISOU39012  O   HOH I 484    4127   3198   3548     60    410    199       O
ATOM  39042  O   HOH I 494      61.261  33.077  80.107  1.00 27.22           O
ANISOU39042  O   HOH I 494    3618   3389   3333     81   -128     61       O
ATOM  39069  O   HOH I 503      76.871  28.406  63.906  1.00 30.69           O
ANISOU39069  O   HOH I 503    4007   3976   3677     -1    227    160       O
ATOM  39186  O   HOH I 542      54.835  12.482  58.354  1.00 23.19           O
ANISOU39186  O   HOH I 542    3262   2611   2937   -213    572    128       O
ATOM  39192  O   HOH I 544      66.833  35.998  76.703  1.00 36.39           O
ANISOU39192  O   HOH I 544    4425   4633   4768     10     37    207       O
ATOM  39348  O   HOH I 596      51.741  33.727  71.143  1.00 31.08           O
ANISOU39348  O   HOH I 596    4166   3803   3838    148   -256      5       O
ATOM  39501  O   HOH I 647      43.892  28.398  64.444  1.00 25.32           O
ANISOU39501  O   HOH I 647    3314   3122   3185    -77    177   -107       O
ATOM  39528  O   HOH I 656      59.610  15.996  62.937  1.00 25.80           O
ANISOU39528  O   HOH I 656    2606   3359   3837    -13    388    183       O
ATOM  39579  O   HOH I 673      60.352  22.045  66.279  1.00 22.69           O
ANISOU39579  O   HOH I 673    2775   2480   3365   -108    -39     54       O
ATOM  39627  O   HOH I 689      75.989  34.827  62.792  1.00 38.42           O
ANISOU39627  O   HOH I 689    5023   4713   4858    299      6     -9       O
ATOM  39666  O   HOH I 702      46.506  18.258  66.442  1.00 39.21           O
ANISOU39666  O   HOH I 702    4778   5310   4809    -43    113    146       O
ATOM  39747  O   HOH I 729      69.594  12.210  67.695  1.00 21.58           O
ANISOU39747  O   HOH I 729    3088   2410   2702   -251     74    354       O
ATOM  39783  O   HOH I 741      42.253  24.456  58.180  1.00 25.06           O
ANISOU39783  O   HOH I 741    2738   3467   3313     33     89    186       O
ATOM  39819  O   HOH I 753      66.393  26.476  65.077  1.00 25.41           O
ANISOU39819  O   HOH I 753    3501   3100   3053    334   -432    144       O
ATOM  39843  O   HOH I 761      55.756  37.559  66.590  1.00 30.32           O
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ANISOU39843	O	HOH	I	761	4217	3354	3949	168	384	-52		O
ATOM	40152	O	HOH	I	864	64.716	14.353	66.359	1.00	27.30		O
ANISOU40152	O	HOH	I	864	3341	3496	3534	-187	-159	341		O
ATOM	40182	O	HOH	I	874	41.524	29.286	67.937	1.00	34.86		O
ANISOU40182	O	HOH	I	874	3934	4683	4628	-179	295	-47		O
ATOM	40191	O	HOH	I	877	60.831	22.658	68.376	1.00	34.79		O
ANISOU40191	O	HOH	I	877	4213	4634	4369	75	35	214		O
ATOM	40248	O	HOH	I	896	64.308	19.693	70.526	1.00	35.61		O
ANISOU40248	O	HOH	I	896	4582	4508	4439	-33	74	-140		O
ATOM	40344	O	HOH	I	928	47.296	24.563	68.734	1.00	31.14		O
ANISOU40344	O	HOH	I	928	3868	4559	3403	114	257	55		O
ATOM	40356	O	HOH	I	932	79.944	21.840	60.235	1.00	29.91		O
ANISOU40356	O	HOH	I	932	3908	3445	4011	86	18	114		O
ATOM	40359	O	HOH	I	933	74.063	26.028	64.165	1.00	29.56		O
ANISOU40359	O	HOH	I	933	3599	3330	4302	-216	-219	-30		O
ATOM	40440	O	HOH	I	960	67.907	44.590	65.913	1.00	25.75		O
ANISOU40440	O	HOH	I	960	3991	3123	2667	307	-94	-102		O
ATOM	40524	O	HOH	I	988	44.680	28.076	71.141	1.00	32.07		O
ANISOU40524	O	HOH	I	988	3615	4563	4007	90	246	71		O
ATOM	40527	O	HOH	I	989	76.881	18.522	65.404	1.00	36.15		O
ANISOU40527	O	HOH	I	989	4732	4581	4420	18	-47	203		O
ATOM	40545	O	HOH	I	995	71.412	31.739	64.211	1.00	37.83		O
ANISOU40545	O	HOH	I	995	5510	4309	4554	-88	-88	-98		O
ATOM	40650	O	HOH	I1030	43.085	35.179	61.829	1.00	29.31			O
ANISOU40650	O	HOH	I1030	3512	4074	3550	-146	328	-25			O
ATOM	40680	O	HOH	I1040	78.792	19.679	63.253	1.00	30.49			O
ANISOU40680	O	HOH	I1040	3304	4489	3791	421	-273	-40			O
ATOM	40743	O	HOH	I1061	62.083	8.368	56.141	1.00	30.31			O
ANISOU40743	O	HOH	I1061	3980	3671	3864	-297	90	139			O
ATOM	41025	O	HOH	I1155	45.685	27.086	64.968	1.00	34.35			O
ANISOU41025	O	HOH	I1155	4377	4478	4196	172	-50	-110			O
ATOM	41028	O	HOH	I1156	65.844	31.135	64.957	1.00	29.31			O
ANISOU41028	O	HOH	I1156	3568	4292	3277	-1	526	71			O
ATOM	41046	O	HOH	I1162	54.204	33.208	71.481	1.00	37.05			O
ANISOU41046	O	HOH	I1162	4197	4861	5018	71	32	-174			O
ATOM	41070	O	HOH	I1170	56.730	27.088	69.870	1.00	26.26			O
ANISOU41070	O	HOH	I1170	3062	3611	3301	106	-323	-47			O
ATOM	41088	O	HOH	I1176	66.289	12.662	67.402	1.00	34.69			O
ANISOU41088	O	HOH	I1176	4168	4266	4745	-147	-209	277			O
ATOM	41241	O	HOH	I1227	42.355	30.902	59.139	1.00	34.91			O
ANISOU41241	O	HOH	I1227	4405	4832	4027	175	327	-244			O
ATOM	41277	O	HOH	I1239	45.815	26.865	68.979	1.00	34.82			O
ANISOU41277	O	HOH	I1239	4752	4483	3995	170	214	-26			O
ATOM	41301	O	HOH	I1247	64.283	33.912	68.802	1.00	33.61			O
ANISOU41301	O	HOH	I1247	4050	4800	3919	-32	124	1			O
ATOM	41328	O	HOH	I1256	74.746	30.073	63.643	1.00	31.66			O
ANISOU41328	O	HOH	I1256	4113	4664	3250	10	118	93			O
ATOM	41361	O	HOH	I1267	46.154	22.723	64.620	1.00	32.16			O
ANISOU41361	O	HOH	I1267	4122	4078	4017	-24	138	-1			O
ATOM	41844	O	HOH	I1428	56.153	44.452	67.899	1.00	68.92			O
ANISOU41844	O	HOH	I1428	8731	8715	8739	43	74	-5			O
ATOM	41931	O	HOH	I1457	42.278	20.775	60.981	1.00	52.15			O
ANISOU41931	O	HOH	I1457	6470	6727	6616	-18	125	-25			O
ATOM	42024	O	HOH	I1488	43.667	25.895	66.993	1.00	49.68			O
ANISOU42024	O	HOH	I1488	6441	6401	6034	29	98	15			O
ATOM	42072	O	HOH	I1504	51.430	29.321	74.525	1.00	43.73			O
ANISOU42072	O	HOH	I1504	5704	5261	5648	116	40	-118			O
ATOM	42189	O	HOH	I1543	63.585	12.662	68.678	1.00	45.50			O
ANISOU42189	O	HOH	I1543	5793	5842	5650	-96	36	39			O
ATOM	42198	O	HOH	I1546	46.149	22.235	68.256	1.00	42.88			O
ANISOU42198	O	HOH	I1546	5244	5352	5696	154	61	74			O

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ATOM  42354  O   HOH I1598      41.897  22.955  60.273  1.00 37.01           O
ANISOU42354  O   HOH I1598    4736   4726   4600   -122    168    -74       O
ATOM  42495  O   HOH I1645      57.936  38.357  70.848  1.00 42.71           O
ANISOU42495  O   HOH I1645    5509   5307   5410    -98    -73     79       O
ATOM  42714  O   HOH I1718      45.890  25.122  63.196  1.00 29.45           O
ANISOU42714  O   HOH I1718    3607   4165   3416   -120    -55    133       O
ATOM  42903  O   HOH I1781      73.809  23.417  69.809  1.00 42.82           O
ANISOU42903  O   HOH I1781    5310   5243   5718    -10     11    -49       O
ATOM  42957  O   HOH I1799      63.112   9.029  60.250  1.00 32.25           O
ANISOU42957  O   HOH I1799    4254   4184   3813    -21    -45    149       O
ATOM  42993  O   HOH I1811      46.174  32.591  72.126  1.00 32.39           O
ANISOU42993  O   HOH I1811    3727   4381   4198    306     54   -215       O
ATOM  43110  O   HOH I1850      59.127  23.677  71.492  1.00 55.65           O
ANISOU43110  O   HOH I1850    7002   6928   7212     21    -54    -64       O
ATOM  43113  O   HOH I1851      50.062  32.026  72.770  1.00 34.54           O
ANISOU43113  O   HOH I1851    4386   4918   3817    187    109   -417       O
ATOM  43176  O   HOH I1872      55.497  43.865  71.656  1.00 49.64           O
ANISOU43176  O   HOH I1872    6514   6169   6175    -22    -13     72       O
ATOM  43227  O   HOH I1889      57.912  37.664  73.936  1.00 40.70           O
ANISOU43227  O   HOH I1889    5242   4982   5239    139     -1    229       O
ATOM  43308  O   HOH I1916      43.859  38.862  61.127  1.00 43.03           O
ANISOU43308  O   HOH I1916    5517   5336   5493     20     26    146       O
ATOM  43551  O   HOH I1997      54.920  12.722  69.483  1.00 50.81           O
ANISOU43551  O   HOH I1997    6663   6316   6326     19    -63     90       O
ATOM  43638  O   HOH I2026      59.575  34.722  67.479  1.00 42.46           O
ANISOU43638  O   HOH I2026    5354   5706   5074   -135    -43    -74       O
ATOM  43677  O   HOH I2039      60.421  28.844  72.145  1.00 46.75           O
ANISOU43677  O   HOH I2039    5824   5960   5975    -81     23     66       O
ATOM  43713  O   HOH I2051      66.641   9.265  60.413  1.00 38.20           O
ANISOU43713  O   HOH I2051    5022   4626   4866     93     40   -255       O
ATOM  43803  O   HOH I2081      68.762  18.925  69.486  1.00 33.71           O
ANISOU43803  O   HOH I2081    4047   4947   3811    127   -107    -57       O
ATOM  43824  O   HOH I2088      50.007  20.442  62.421  1.00 39.29           O
ANISOU43824  O   HOH I2088    5208   4899   4820   -187    276     96       O
ATOM  43872  O   HOH I2104      43.901  18.608  62.146  1.00 30.97           O
ANISOU43872  O   HOH I2104    3623   4213   3929   -106    378    -62       O
ATOM  43896  O   HOH I2112      59.270  31.554  78.642  1.00 45.34           O
ANISOU43896  O   HOH I2112    5475   6003   5749     27    -97   -112       O
ATOM  43899  O   HOH I2113      75.848  33.861  66.101  1.00 39.65           O
ANISOU43899  O   HOH I2113    4880   5004   5179    -85    -88   -152       O
ATOM  43902  O   HOH I2114      44.759  22.939  71.345  1.00 50.34           O
ANISOU43902  O   HOH I2114    6343   6307   6478    -67      9     95       O
ATOM  43962  O   HOH I2134      54.344  35.938  72.158  1.00 51.31           O
ANISOU43962  O   HOH I2134    6457   6482   6556     33    -16     13       O
ATOM  44097  O   HOH I2179      71.025  19.374  71.132  1.00 28.30           O
ANISOU44097  O   HOH I2179    3671   4038   3042     21    -26    -98       O
ATOM  44223  O   HOH I2221      65.453  37.557  58.489  1.00 43.47           O
ANISOU44223  O   HOH I2221    5582   5436   5498   -196   -181     40       O
ATOM  44226  O   HOH I2222      73.226  32.771  73.023  1.00 64.60           O
ANISOU44226  O   HOH I2222    8146   8188   8209     75     20    -52       O
ATOM  44265  O   HOH I2235      59.055  12.618  63.231  1.00 52.50           O
ANISOU44265  O   HOH I2235    6807   6614   6527    -99    -75    -77       O
ATOM  44280  O   HOH I2240      59.423  25.674  68.487  1.00 42.74           O
ANISOU44280  O   HOH I2240    5486   5223   5530     15   -156     23       O
ATOM  44394  O   HOH I2278      66.931  20.767  70.911  1.00 37.52           O
ANISOU44394  O   HOH I2278    4654   5168   4433   -325    232    121       O
ATOM  44547  O   HOH I2329      56.302  11.513  62.665  1.00 34.16           O
ANISOU44547  O   HOH I2329    4405   4218   4355     45     89    -33       O
ATOM  44589  O   HOH I2343      67.682  41.065  69.985  1.00 52.46           O
ANISOU44589  O   HOH I2343    6488   6755   6687     39     71     78       O
ATOM  44688  O   HOH I2376      42.482  36.027  58.782  1.00 33.76           O
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ANISOU44688  O   HOH I2376     3344   4897   4584   -343    -25    131      O
ATOM  45057  O   HOH I2499      62.441  25.697  68.988  1.00 43.45           O
ANISOU45057  O   HOH I2499     5410   5569   5527     18     73    -47      O
ATOM  45210  O   HOH I2550      64.664  24.898  70.613  1.00 63.32           O
ANISOU45210  O   HOH I2550     8101   7967   7989      0    -17     35      O
ATOM  45216  O   HOH I2552      61.609  27.647  69.632  1.00 52.86           O
ANISOU45216  O   HOH I2552     6647   6624   6813    -95    -59     12      O
ATOM  45222  O   HOH I2554      51.446  12.951  63.313  1.00 32.89           O
ANISOU45222  O   HOH I2554     4197   4003   4294   -174     26    163      O
ATOM  45255  O   HOH I2565      73.299  17.756  70.832  1.00 46.42           O
ANISOU45255  O   HOH I2565     6056   5769   5810     41   -105    -68      O
ATOM  45450  O   HOH I2630      67.830  23.507  69.574  1.00 47.33           O
ANISOU45450  O   HOH I2630     5827   6179   5977    -97     93     10      O
ATOM  45507  O   HOH I2649      56.545  41.609  72.147  1.00 45.80           O
ANISOU45507  O   HOH I2649     5565   5761   6076    122     69    -71      O
ATOM  45528  O   HOH I2656      68.079  24.630  73.000  1.00 43.47           O
ANISOU45528  O   HOH I2656     5390   5451   5676     -7   -101    -16      O
ATOM  45546  O   HOH I2662      53.203  15.494  71.706  1.00 47.73           O
ANISOU45546  O   HOH I2662     5931   6247   5956    -97    127     17      O
ATOM  45552  O   HOH I2664      72.139  26.355  70.120  1.00 66.65           O
ANISOU45552  O   HOH I2664     8433   8375   8515    -35     19     20      O
ATOM  45585  O   HOH I2675      49.569  28.163  74.878  1.00 49.85           O
ANISOU45585  O   HOH I2675     6262   6313   6365     64    -43    -38      O
ATOM  45603  O   HOH I2681      56.406  11.065  60.146  1.00 33.83           O
ANISOU45603  O   HOH I2681     4194   4022   4638    -69     63    -24      O
ATOM  45633  O   HOH I2691      51.596  30.097  77.007  1.00 60.68           O
ANISOU45633  O   HOH I2691     7748   7631   7674    -37      0      3      O
ATOM  45717  O   HOH I2719      72.738  28.983  68.543  1.00 63.69           O
ANISOU45717  O   HOH I2719     8078   8045   8075     -1    -16     11      O
ATOM  45933  O   HOH I2791      72.650  24.936  61.880  1.00 45.51           O
ANISOU45933  O   HOH I2791     5697   5825   5768     59    -36    -33      O
ATOM  45996  O   HOH I2812      52.245  43.052  72.881  1.00 45.38           O
ANISOU45996  O   HOH I2812     5728   5866   5645      1    -15    -10      O
ATOM  46086  O   HOH I2842      70.833  22.382  70.704  1.00 46.92           O
ANISOU46086  O   HOH I2842     6084   6103   5640    111     22   -116      O
ATOM  46140  O   HOH I2860      76.101  31.721  63.074  1.00 51.42           O
ANISOU46140  O   HOH I2860     6715   6574   6246    -49     37    -20      O
ATOM  46203  O   HOH I2881      60.875   9.923  69.241  1.00 39.15           O
ANISOU46203  O   HOH I2881     4976   4735   5161    163      3     42      O
ATOM  46215  O   HOH I2885      62.072  14.845  70.562  1.00 48.90           O
ANISOU46215  O   HOH I2885     6005   6257   6315    -52     40     56      O
ATOM  46224  O   HOH I2888      67.153  17.681  74.494  1.00 53.05           O
ANISOU46224  O   HOH I2888     6670   6759   6726    -88      3      9      O
ATOM  46242  O   HOH I2894      50.382  35.259  75.028  1.00 46.75           O
ANISOU46242  O   HOH I2894     5778   6146   5837     90     43    115      O
ATOM  46251  O   HOH I2897      74.189  32.497  68.445  1.00 50.96           O
ANISOU46251  O   HOH I2897     6676   6134   6552    -61    -48     30      O
ATOM  46266  O   HOH I2902      51.944  36.711  76.282  1.00 61.13           O
ANISOU46266  O   HOH I2902     7753   7682   7792      2     43      9      O
ATOM  46275  O   HOH I2905      68.307  19.936  76.278  1.00 48.19           O
ANISOU46275  O   HOH I2905     5964   6205   6139     82    -21    -70      O
ATOM  46341  O   HOH I2927      61.473  15.804  72.791  1.00 67.70           O
ANISOU46341  O   HOH I2927     8549   8524   8646     17    -44    -11      O
ATOM  46347  O   HOH I2929      70.087  28.966  70.429  1.00 51.54           O
ANISOU46347  O   HOH I2929     6629   6422   6531    -79     33     31      O
ATOM  46452  O   HOH I2964      59.644  24.439  65.361  1.00 24.35           O
ANISOU46452  O   HOH I2964     2799   2670   3782    119   -492    114      O
ATOM  46455  O   HOH I2965      65.407  28.461  63.629  1.00 35.39           O
ANISOU46455  O   HOH I2965     4437   4538   4469    266   -368   -260      O
ATOM  46470  O   HOH I2970      63.893  29.687  62.345  1.00 34.97           O
ANISOU46470  O   HOH I2970     4714   4317   4255     52    139    190      O
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ATOM  46509  O   HOH I2983      57.732  30.602  70.029  1.00 52.81           O
ANISOU46509  O   HOH I2983    6628   6700   6735    -67    -44     22        O
ATOM  46512  O   HOH I2984      63.472  29.428  73.612  1.00 43.98           O
ANISOU46512  O   HOH I2984    5677   5542   5491    -46     -1     88        O
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Claims

1. A method of selecting agents which inhibit the enzyme glucose-1-phosphate thymidylyltransferase (RmlA), said method comprising the steps of:

a) providing a model of the active or regulatory site(s) of RmlA;

b) reviewing the structure of a potential inhibitory agent for at least one of these sites; and

c) analysing the potential interaction of said agent in said site(s).

2. A method as claimed in Claim 1 further including the step of selecting an agent which interacts with the active or regulatory site(s) of RmlA.

3. The method as claimed in Claim 2 wherein said agent binds to the active or regulatory site(s) of RmlA sufficiently tightly to impede the biosynthesis of rhamnose.

4. The method as claimed in either one of Claims 2 and 3 wherein said agent has a negative charge which interacts with Arg 15 and/or Lys 25 of RmlA.

5. The method as claimed in either one of Claims 2 and 3 wherein said agent has a thymidyl-like moiety able to interact with Gly 10, Gln 82 and/or Gly 87 of RmlA.

6. The method as claimed in Claim 5 wherein said thymidyl-like moiety forms a hydrogen bond with Gly 10, Gln 82 and/or Gly 87 of RmlA.

7. The method as claimed in either one of Claims 2 and 3 wherein said agent has a glucose-like moiety able to interact with Asn 111, Gly 146, Glu 161, Val 172 and/or Thr 176 of RmlA.

8. The method as claimed in Claim 7 wherein said glucose-like moiety forms a hydrogen bond with Asn 111, Gly 146, Glu 161, Val 172 and/or Thr 176 of RmlA.

9. The method as claimed in any one of Claims 1 to 8 wherein said model of RmlA is in the form of a computer data file.

10. The method as claimed in any one of Claims 1 to 9 wherein said model is based upon the X-ray crystal co-ordinates of RmlA.

11. The method as claimed in Claim 10 wherein said model includes the data for the regulatory site(s) as set out in Annex 1.

12. The method as claimed in Claim 10 wherein said model includes the data for the active site(s) as set out in Annex 2.

13. The method as claimed in any one of Claims 1 to 12 wherein step b) includes providing a model of the potential inhibitory agent.

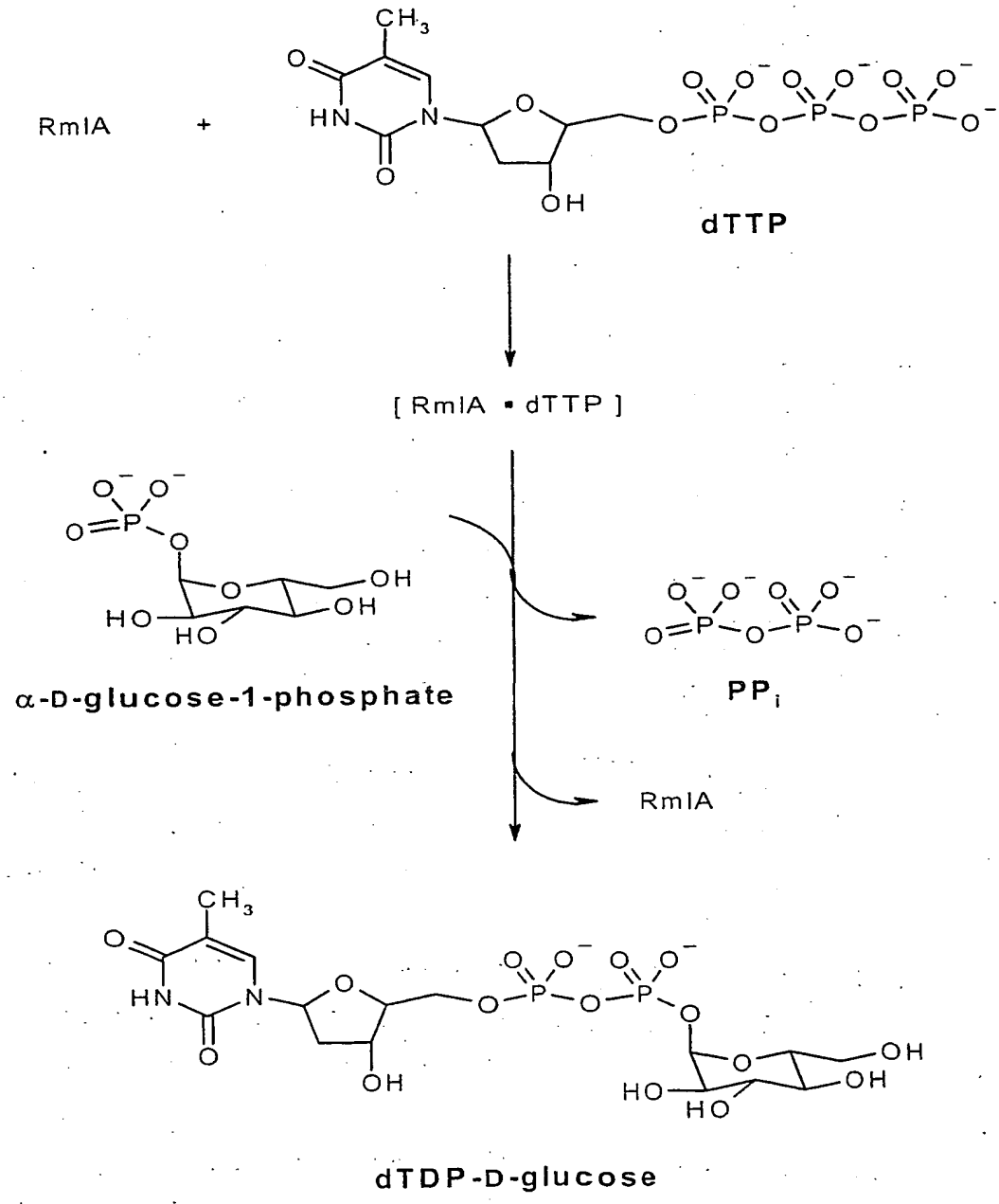
14. The method as claimed in Claim 13 wherein said model is in the form of a computer data file.

15. The method as claimed in any one of Claims 1 to 14 wherein the intermolecular interaction between said agent and the model of the active or regulatory site(s) of RmlA is analysed with the aid of a computer.

16. A purified and crystallised form of the enzyme glucose-1-phosphate thymidylyltransferase (RmlA) obtained from *Pseudomonas aeruginosa*.

17. Use of the purified and crystallised form of RmlA as claimed in Claim 16 to select for inhibitors of said enzyme.

18. Use as claimed in Claim 17 wherein said inhibitors inhibit the growth of *Pseudomonas aeruginosa*.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+
dTTP
[RmlA • dTTP]
α-D-glucose-1-phosphate
PPi
RmlA
dTDP-D-glucose

Figure 1

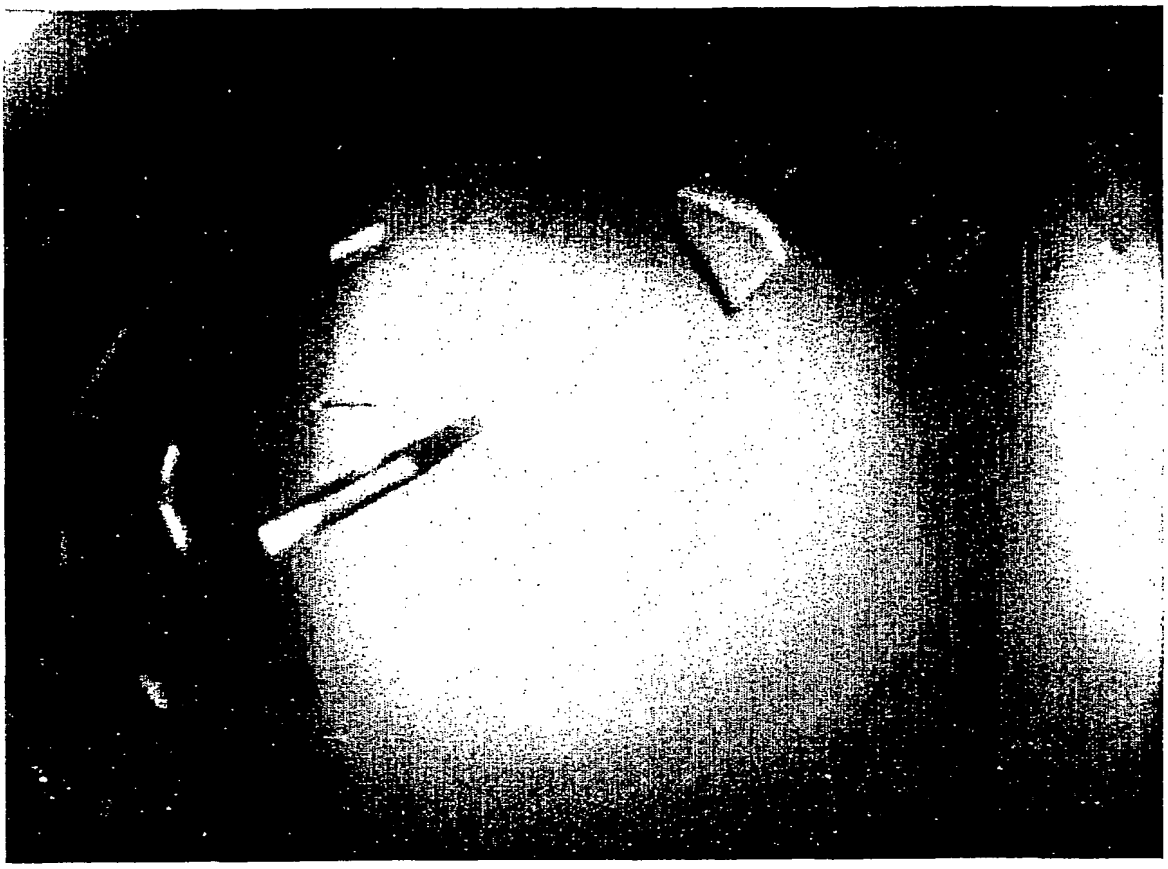


Figure 2

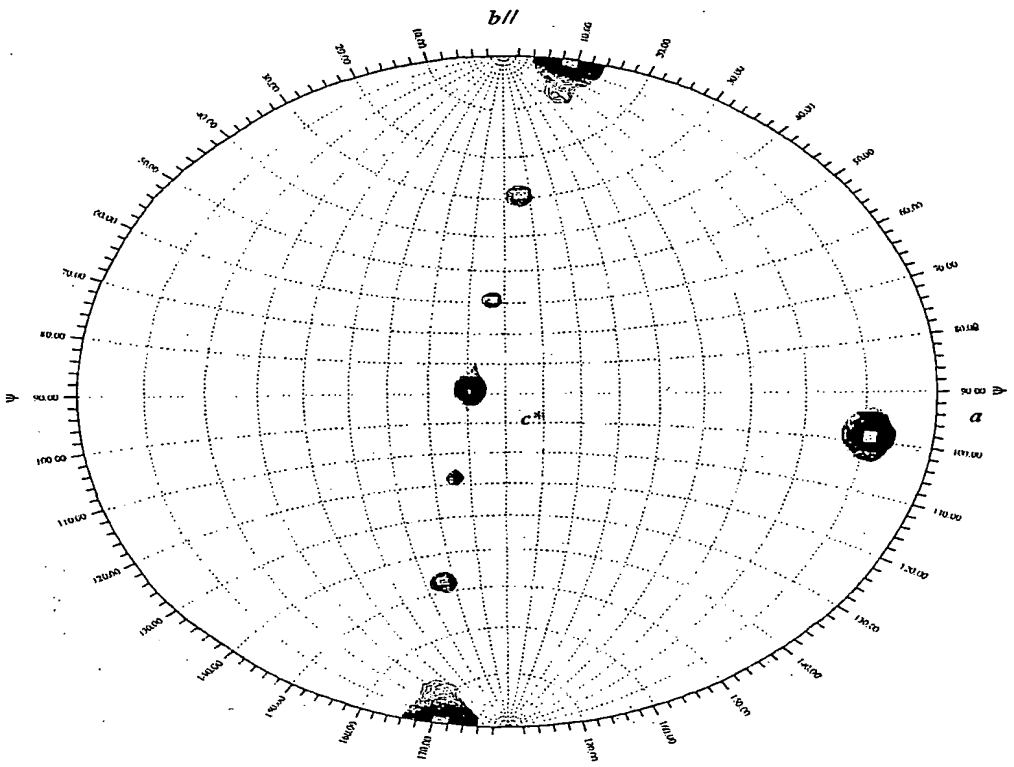


Figure 3

Table 1. Data collection statistics for non-Se-labelled RmlA crystals

Values in parentheses refer to the highest shell.

Crystal grown in the presence of	Glucose-1-phosphate (G1P)	Glucose-1-phosphate	dTDP-glucose	G1P/thymidine/AlF_3	dTMP
X-Ray source	rotating anode	ID14EH1	ID14EH1	ID14EH1	BM14
Wavelength (Å)	1.542	0.934	0.934	0.934	0.978
Resolution (Å)	36.27 – 2.27 (2.40 – 2.27)	40.49 – 1.90 (1.99 – 1.90)	40.49 – 1.77 (1.86 – 1.77)	36.27 – 1.87 (1.97 – 1.87)	32.12 – 1.66 (1.74 – 1.66)
Unit cell (Å; °)	a=71.6, b=73.5, c=134.2; α=89.9, β=80.8, δ=80.8	a=71.7, b=73.7, c=134.5; α=90.0, β=80.9, δ=80.9	a=71.6, b=73.4, c=134.3; α=89.9, β=80.6, δ=80.9	a=71.3, b=73.1, c=133.7; α=90.0, β=81.4, δ=81.6	a=71.5, b=73.1, c=134.7; α=89.9, β=80.9, δ=81.1
V_m ($Å^3$/Da)	2.55	2.56	2.54	2.52	2.54
Total measurements	305802	377690	483036	333697	1141819
Unique reflections	116157	202988	242450	183207	297160
I/σ	6.8 (4.8)	9.2 (1.9)	7.1 (2.4)	6.9 (2.4)	10.9 (2.0)
Average redundancy	2.6 (2.3)	1.9 (1.9)	2.0 (1.3)	1.8 (1.3)	3.8 (2.0)
Completeness (%)	94.2 (84.2)	96.1 (95.6)	93.9 (77.4)	84.7 (66.8)	94.2 (81.2)
R_{merge} (%) †	6.5 (15.2)	5.4 (28.6)	7.2 (30.2)	6.7 (29.1)	5.3 (33.2)

† $R_{merge} = \sum\sum I(h)_j - \langle I(h) \rangle / \sum\sum I(h)_j$ *where I(h) is the measured diffraction intensity and the summation includes all observations.*

Figure 4

Table 2. Data collection statistics for MAD experiment on BM14 (ESRF-Grenoble)

Values in parentheses refer to the highest shell.

Position	Peak	Inflection	Remote
Wavelength (Å)	0.9790	0.9791	0.8855
Resolution (Å)	30.0 – 2.8 (2.87 – 2.80)		
Unit cell (Å; °)	a=71.6, b=73.9, c=133.8; α=89.8, β=80.3, δ=80.2		
V_m (Å^3/Da)	2.54		
Total measurements	221219	220585	224654
Unique reflections	121843	121982	121112
I/σ	31.7 (9.0)	31.6 (8.8)	29.7 (9.8)
Average redundancy	1.8 (1.0)	1.8 (1.0)	1.9 (1.7)
Completeness (%)	93.0 (63.2)	93.0 (63.2)	92.7 (69.4)
R_{merge} (%) †	2.2 (8.9)	2.3 (9.5)	2.4 (8.9)

† $R_{\text{-merge}} = \Sigma\Sigma I(h)_j - \langle I(h)\rangle / \Sigma\Sigma I(h)_j$ *where I(h) is the measured diffraction intensity and the summation includes all observations.*

Figure 5

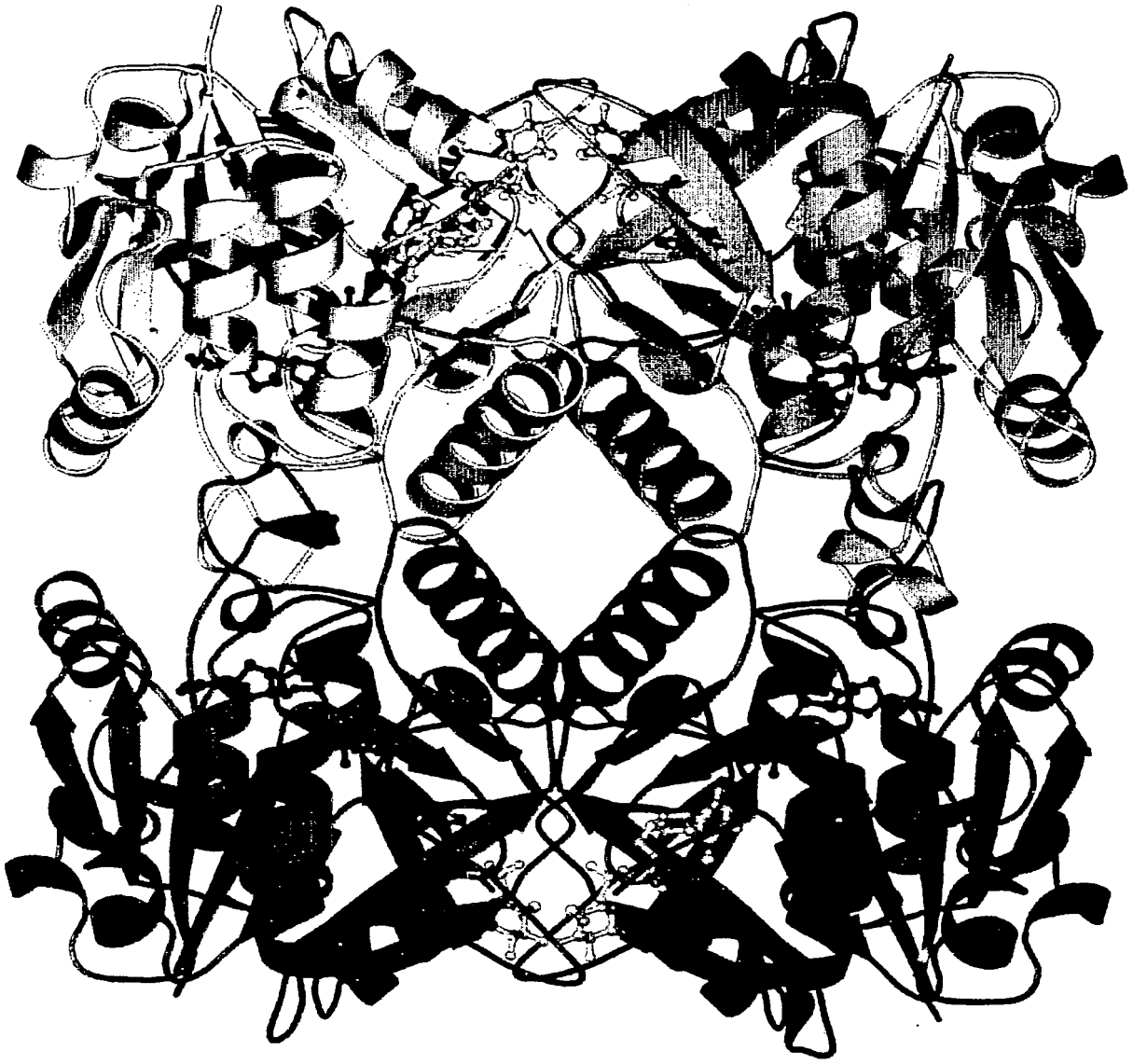
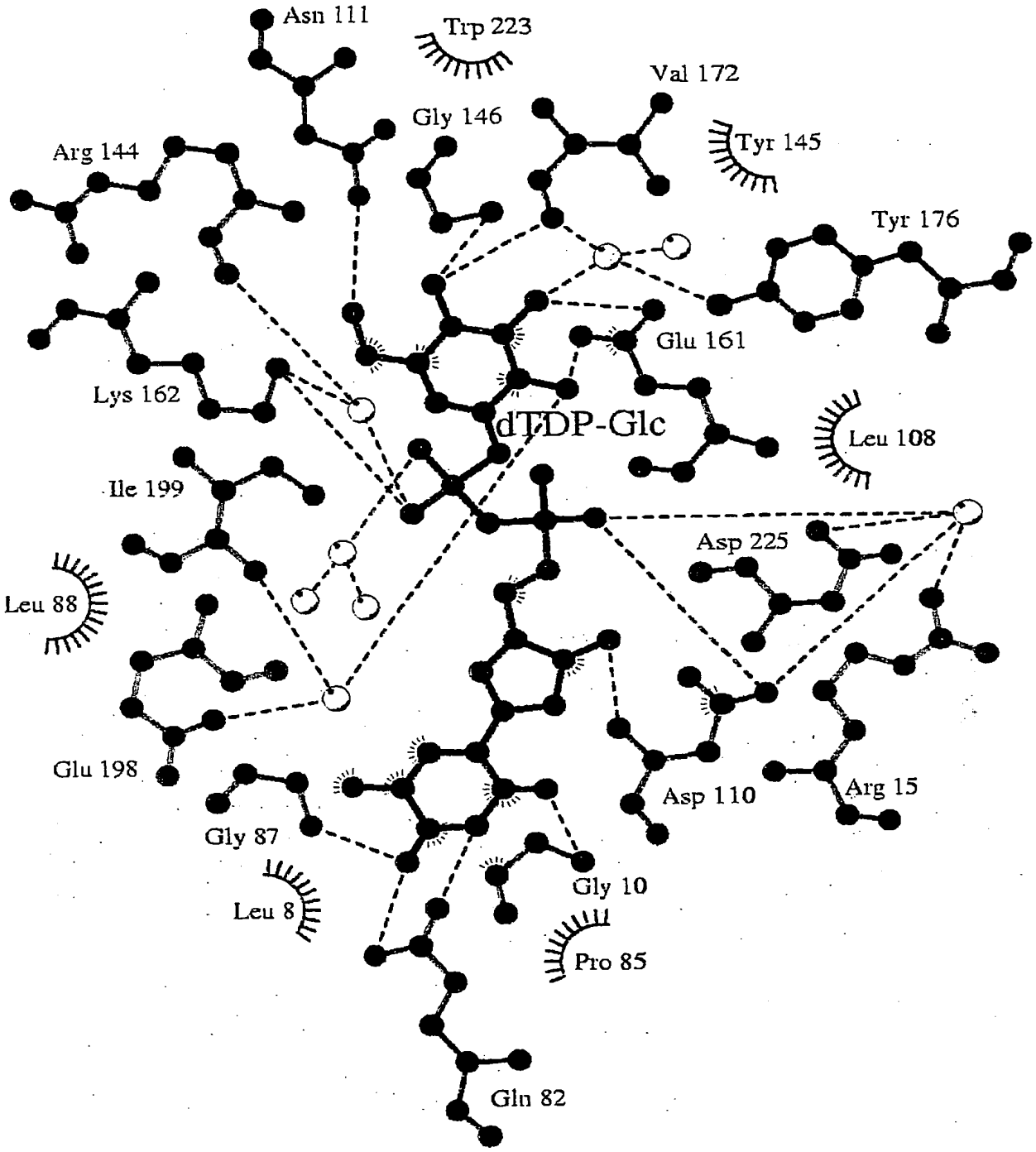


Fig. 6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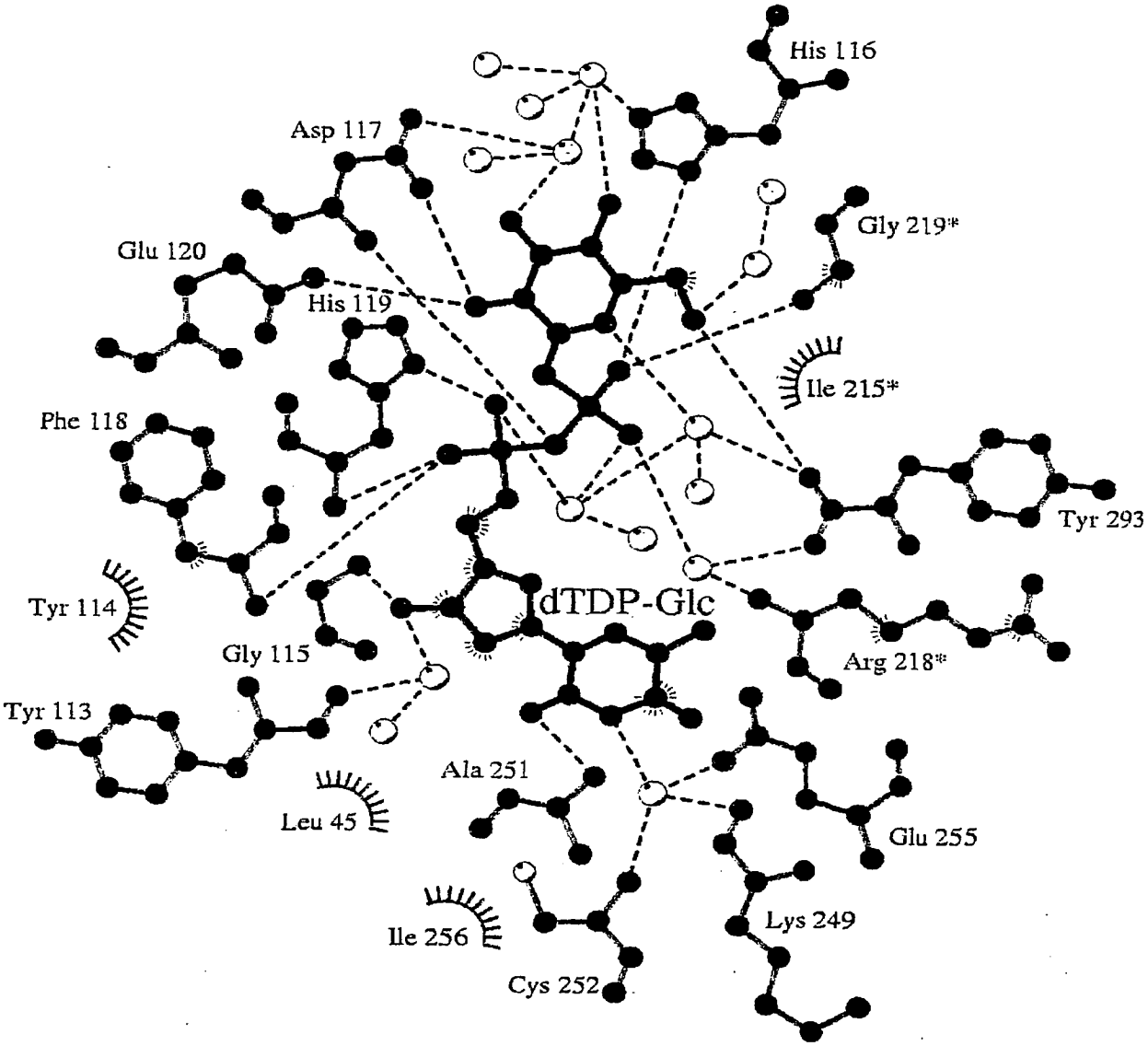
Trp 223
Val 172
Gly 146
Tyr 145
Arg 144
Tyr 176
Glu 161
Lys 162
dTDP-Glc
Leu 108
Ile 199
Asp 225
Leu 88
Glu 198
Asp 110
Arg 15
Gly 87
Gly 10
Leu 8
Pro 85
Gln 82

Fig. 7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Glu 120
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Tyr 293
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Tyr 113
Ala 251
Leu 45
Glu 255
Lys 249
Ile 256
Cys 252

Fig. 8

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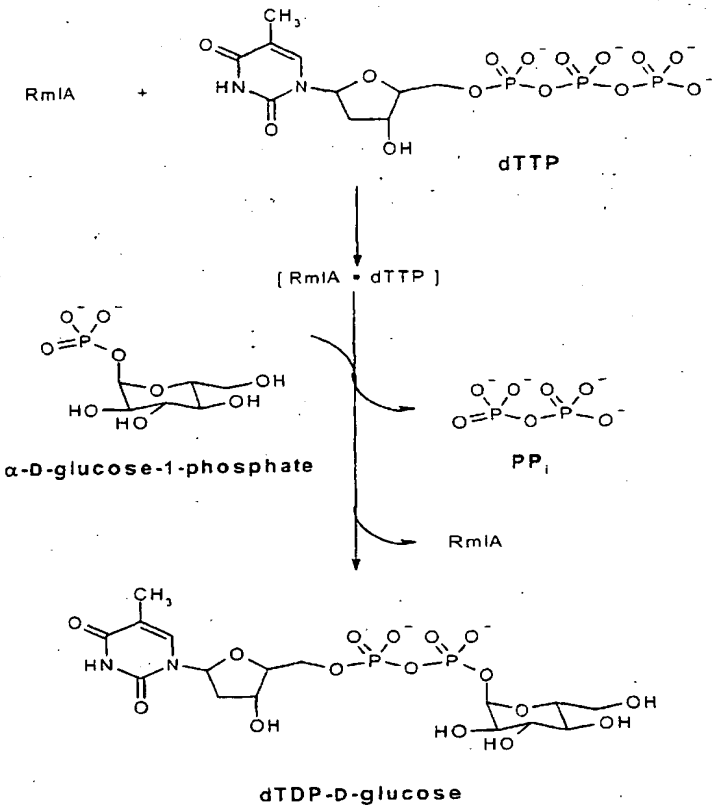
[Continued on next page]

(54) Title: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE AND METHOD FOR SELECTING INHIBITORS THEREOF



(57) Abstract: There is provided a method of obtaining selecting agents which inhibit the enzyme glucose-1-phosphate thymidylyl-transferase (RmlA) based upon analysis of a model of the active and regulatory site (s) of RmlA and interaction therewith by a potential inhibitory agent. The invention is based upon the provision of information on the structure of RmlA obtained through X-ray diffraction studies since a crystallised form of RmlA was obtained for the first time. The purified and crystallised from of RmlA, obtained from *Psemdomononas aeruginosa* is also described.

WO 02/006509 A3

patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

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PCT/GB 01/03152

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According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
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Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)
CHEM ABS Data, MEDLINE, BIOSIS, EPO-Internal, WPI Data, PAJ

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	MA, YUFANG ET AL: "Determination of the pathway for rhamnose biosynthesis in mycobacteria: cloning, sequencing and expression of the Mycobacterium tuberculosis gene encoding.alpha.-D-glucose-1- phosphate thymidylyltransferase" MICROBIOLOGY (READING, U. K.) (1997), 143(3), 937-945 , XP008003838 the whole document --- -/--	1,16

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Date of the actual completion of the international search	Date of mailing of the international search report
6 June 2002	17/06/2002

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Moreno, C

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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	BLANKENFELDT W ET AL: "The structural basis of the catalytic mechanism and regulation of glucose-1-phosphate thymidylyltransferase (RmlA)" THE EMBO JOURNAL , vol. 19, no. 24, 2000, pages 6652-6663, XP001074715 abstract ---	1-18
P,X	BLANKENFELDT, WULF ET AL: "The purification, crystallization and preliminary structural characterization of glucose-1-phosphate thymidylyltransferase (RmlA), the first enzyme of the dTDP-L-rhamnose synthesis pathway from Pseudomonas aeruginosa" ACTA CRYSTALLOGRAPHICA, SECTION D: BIOLOGICAL CRYSTALLOGRAPHY (2000), D56(11), 1501-1504 , XP008003837 abstract -----	1,16